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| | | | |
|------|----|--------|--|
| NEWS | 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS | 2 | AUG 06 | CAS REGISTRY enhanced with new experimental property tags |
| NEWS | 3 | AUG 06 | FSTA enhanced with new thesaurus edition |
| NEWS | 4 | AUG 13 | CA/Capplus enhanced with additional kind codes for granted patents |
| NEWS | 5 | AUG 20 | CA/Capplus enhanced with CAS indexing in pre-1907 records |
| NEWS | 6 | AUG 27 | Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB |
| NEWS | 7 | AUG 27 | USPATOLD now available on STN |
| NEWS | 8 | AUG 28 | CAS REGISTRY enhanced with additional experimental spectral property data |
| NEWS | 9 | SEP 07 | STN AnaVist, Version 2.0, now available with Derwent World Patents Index |
| NEWS | 10 | SEP 13 | FORIS renamed to SOFIS |
| NEWS | 11 | SEP 13 | INPADOCDB enhanced with monthly SDI frequency |
| NEWS | 12 | SEP 17 | CA/Capplus enhanced with printed CA page images from 1967-1998 |
| NEWS | 13 | SEP 17 | Caplus coverage extended to include traditional medicine patents |
| NEWS | 14 | SEP 24 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS | 15 | OCT 02 | CA/Capplus enhanced with pre-1907 records from Chemisches Zentralblatt |
| NEWS | 16 | OCT 19 | BEILSTEIN updated with new compounds |
| NEWS | 17 | NOV 15 | Derwent Indian patent publication number format enhanced |
| NEWS | 18 | NOV 19 | WPIX enhanced with XML display format |
| NEWS | 19 | NOV 30 | ICSD reloaded with enhancements |
| NEWS | 20 | DEC 04 | LINPADOCDB now available on STN |
| NEWS | 21 | DEC 14 | BEILSTEIN pricing structure to change |
| NEWS | 22 | DEC 17 | USPATOLD added to additional database clusters |
| NEWS | 23 | DEC 17 | IMSDRUGCONF removed from database clusters and STN |
| NEWS | 24 | DEC 17 | DGENE now includes more than 10 million sequences |
| NEWS | 25 | DEC 17 | TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment |
| NEWS | 26 | DEC 17 | MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary |
| NEWS | 27 | DEC 17 | CA/Capplus enhanced with new custom IPC display formats |
| NEWS | 28 | DEC 17 | STN Viewer enhanced with full-text patent content from USPATOLD |
| NEWS | 29 | JAN 02 | STN pricing information for 2008 now available |
| NEWS | 30 | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS | 31 | JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS | 32 | JAN 28 | MARPAT searching enhanced |
| NEWS | 33 | JAN 28 | USGENE timeliness enhanced |
| NEWS | 34 | JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS | 35 | JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements |

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,

CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

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|----------------------|---------------------|------------------|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 18:19:31 ON 28 JAN 2008

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DICTIONARY FILE UPDATES: 27 JAN 2008 HIGHEST RN 1000849-38-6

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=>

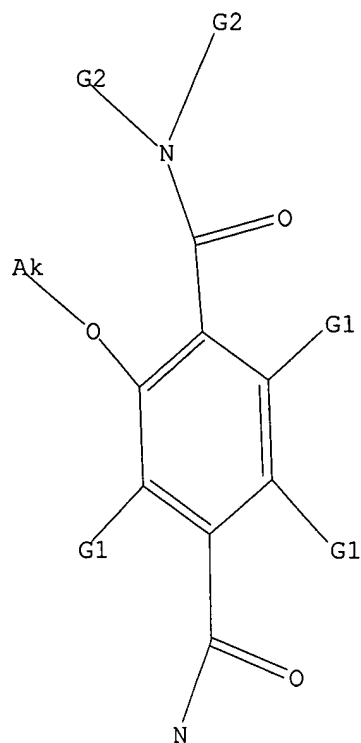
Uploading C:\Documents and Settings\jcho2\My Documents\10588478-c.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 C,H,S,N

G2 H,Ak,NH,NH2

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 18:19:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3389 TO ITERATE

100.0% PROCESSED 3389 ITERATIONS

196 ANSWERS

SEARCH TIME: 00.00.01

L2 196 SEA SSS FUL L1

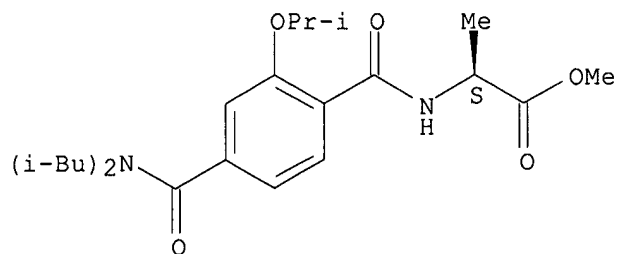
=> d scan

L2 196 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester

MF C23 H36 N2 O5

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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178.57

FILE 'CAPLUS' ENTERED AT 18:20:09 ON 28 JAN 2008

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FILE COVERS 1907 - 28 Jan 2008 VOL 148 ISS 5

FILE LAST UPDATED: 27 Jan 2008 (20080127/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 12

L3 28 L2

=> d 13 1-17 bib abs hitstr

L3 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:63581 CAPLUS

DN 146:156259

TI MAO-B inhibitors useful for treating obesity

IN McElroy, John F.; Chorvat, Robert J.; Rajagopalan, Parthasarathi

PA Jenrin Discovery, USA

SO PCT Int. Appl., 92pp.

CODEN: PIXXD2

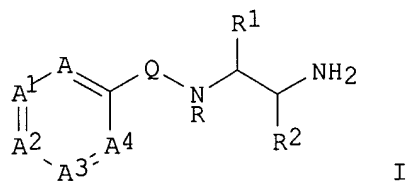
DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| | ----- | ---- | ----- | ----- | ----- |
| PI | WO 2007008963 | A1 | 20070118 | WO 2006-US27019 | 20060712 |
| | W: | | | | |
| | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, | | | | |
| | CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, | | | | |
| | GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, | | | | |
| | KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, | | | | |
| | MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, | | | | |
| | SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, | | | | |
| | US, UZ, VC, VN, ZA, ZM, ZW | | | | |
| | RW: | | | | |
| | AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, | | | | |
| | IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, | | | | |
| | CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, | | | | |

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM
 US 2007015734 A1 20070118 US 2006-456912 20060712
 PRAI US 2005-698867P P 20050713
 OS MARPAT 146:156259
 GI

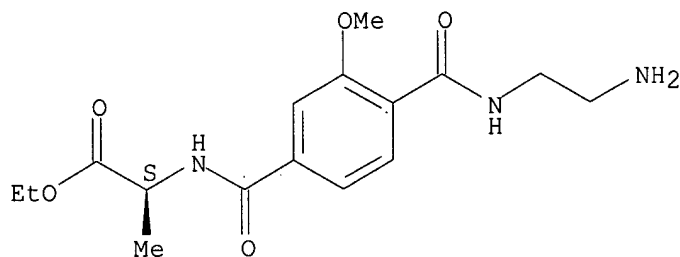


AB The invention provides novel compds. of formula I (where A, A1, A2, A3, and A4, are independently selected from CH, substituted C, N, and N+-O-, provided that from 0-1 is N+-O-; R is independently selected from H and C1-6 alkyl; R1 is selected from H and C1-6 alkyl; R2 is selected from H and C1-6-alkyl; Q is selected from C=O and SO2) that are monoamine oxidase-B (MAO-B) inhibitors, which can be useful in treating obesity, diabetes, and/or cardiometabolic disorders (e.g., hypertension, dyslipidemias, high blood pressure, and insulin resistance).

IT 919772-32-0 919772-33-1 919772-34-2
 919772-35-3
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (MAO-B inhibitors useful for treating obesity and other disorders)

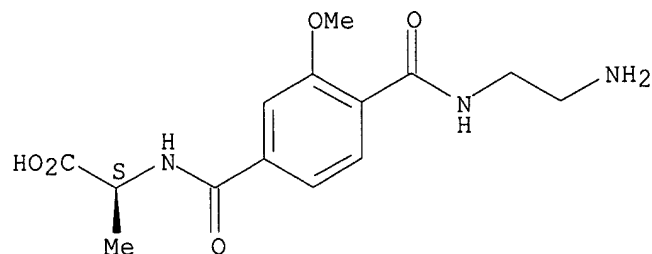
RN 919772-32-0 CAPLUS
 CN L-Alanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



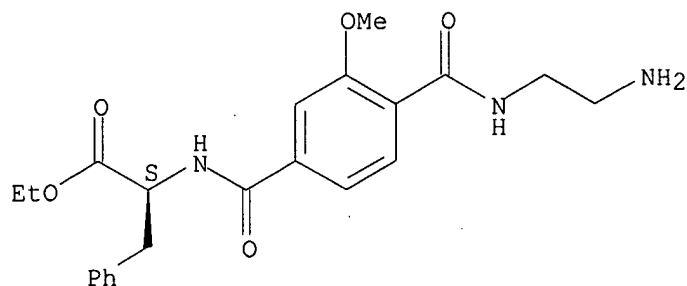
RN 919772-33-1 CAPLUS
 CN L-Alanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



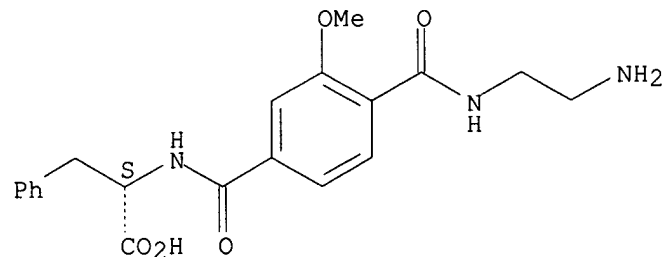
RN 919772-34-2 CAPLUS
CN L-Phenylalanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 919772-35-3 CAPLUS
CN L-Phenylalanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.

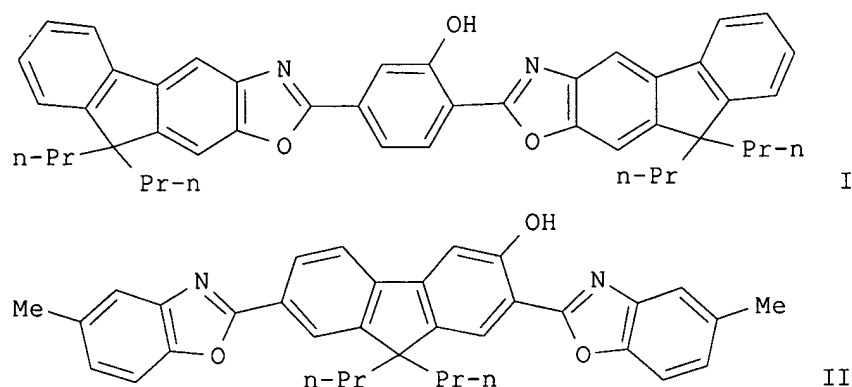


RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:656393 CAPLUS
DN 145:124546
TI Preparation of benzoxazole derivatives for the manufacture of ophthalmic lenses
IN Kauffman, Joeel; Litak, Peter T.; Rickwood, Martin
PA Essilor International (Compagnie Generale D'Optique), Fr.
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----|--|------|----------|-----------------|----------|
| PI | WO 2006069811 | A2 | 20060706 | WO 2005-EP14202 | 20051230 |
| | WO 2006069811 | A3 | 20070104 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: | AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, | | | | |

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM
 AU 2005321406 A1 20060706 AU 2005-321406 20051230
 CA 2592585 A1 20060706 CA 2005-2592585 20051230
 EP 1838682 A2 20071003 EP 2005-850391 20051230
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRAI US 2004-640506P P 20041230
 WO 2005-EP14202 W 20051230
 OS MARPAT 145:124546
 GI



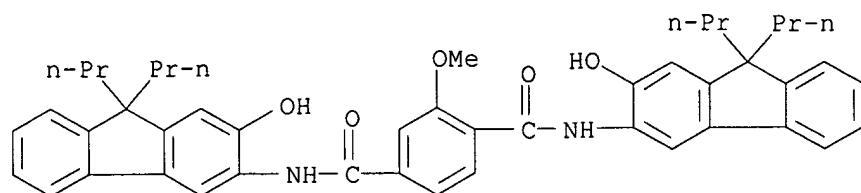
AB Compds. that absorb UV light 380 nm to 400 nm range but avoid absorption in the blue light range, thereby imparting yellowness, i.e., 410-420 nm have suitable refractive characteristics useful in the preparation of optical resins or plastics suitable, for example, for the manufacture of ophthalmic lenses. Methods for making the compds. I and II, which were prepared in a multi-step synthesis starting from 2-methoxyterephthalic acid and 3-methoxyfluorene resp., optic lenses containing the compds., and methods for making these are also described.

IT 897364-45-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 9H-fluoreno[3,2-d]oxazole and benzoxazolyfluorene derivs. as optical lenses)

RN 897364-45-3 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis(2-hydroxy-9,9-dipropyl-9H-fluoren-3-yl)-2-methoxy- (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:127910 CAPLUS

DN 144:378247

TI Synthesis and characterization of new electroluminescent molecules

containing carbazole and oxadiazole units

AU Bugatti, Valeria; Concilio, Simona; Iannelli, Pio; Piotto, Stefano P.; Bellone, Salvatore; Ferrara, Manuela; Neitzert, Heinrich C.; Rubino, Alfredo; Della Sala, Dario; Vacca, Paolo

CS Dipartimento di Ingegneria Chimica ed Alimentare, Universita di Salerno, Fisciano (Salerno), I-84084, Italy

SO Synthetic Metals (2006), 156(1), 13-20
CODEN: SYMEDZ; ISSN: 0379-6779

PB Elsevier B.V.

DT Journal

LA English

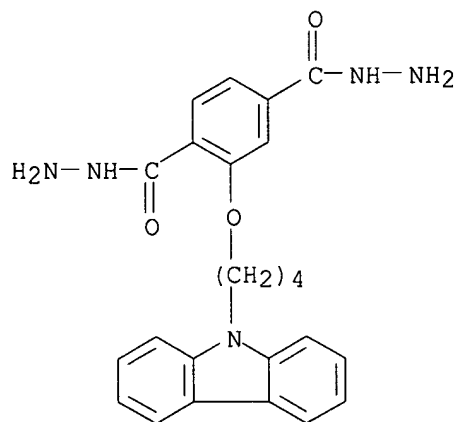
OS CASREACT 144:378247

AB The synthesis of new mols. containing both electron and hole transporter units is reported. This class of compds., named OC, may be used for assembling electroluminescent devices made by a single organic layer. The active moieties are the carbazole, as the hole transporter unit, and the oxadiazole, as the electron transporter unit. The chemical formulation and the complex geometry of the mol. frame allow good solubility in chlorinated solvents and the preparation of homogeneous films by spinning technique. Photoluminescence of mols., both in solution and in film, occurs in the blue region of visible spectra, the exact peak position of emission depending on the pendants attached to the oxadiazole unit. The electroluminescence occurs in a higher wavelength region, with a blue-green emission. The electroluminescent devices consist in the simple sequence ITO-OC-Al and ITO-PEDOT-OC-Al.

IT 881896-43-1P 881896-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzoylation; synthesis of electroluminescent mols. containing carbazole hole transport and oxadiazole electron transport units for a single-layer blue-emitting OLED)

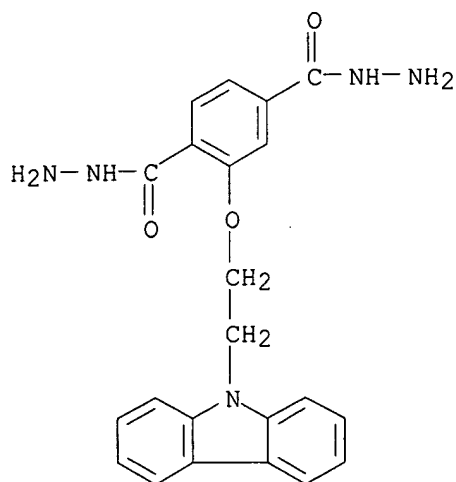
RN 881896-43-1 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-, dihydrazide (9CI) (CA INDEX NAME)



RN 881896-44-2 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[2-(9H-carbazol-9-yl)ethoxy]-, dihydrazide (9CI) (CA INDEX NAME)

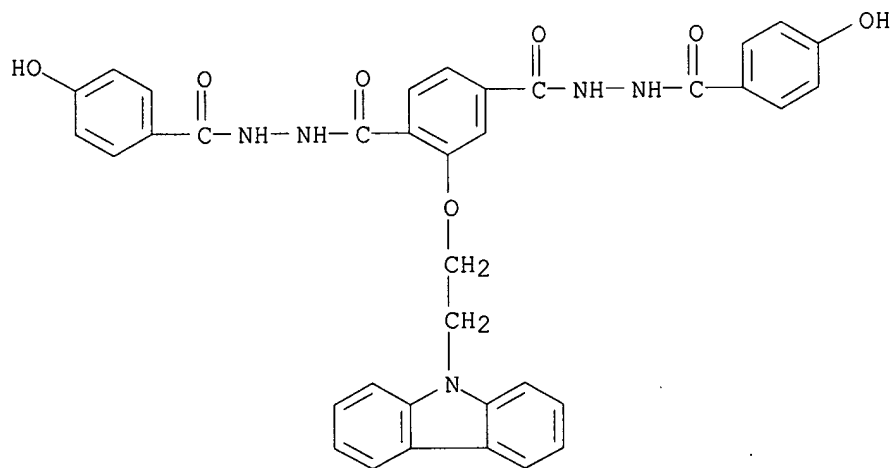


IT 881896-45-3P 881896-46-4P 881896-47-5P
881896-48-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(intramol. cyclization and thermal data; synthesis of
electroluminescent mols. containing carbazole hole transport and oxadiazole
electron transport units for a single-layer blue-emitting OLED)

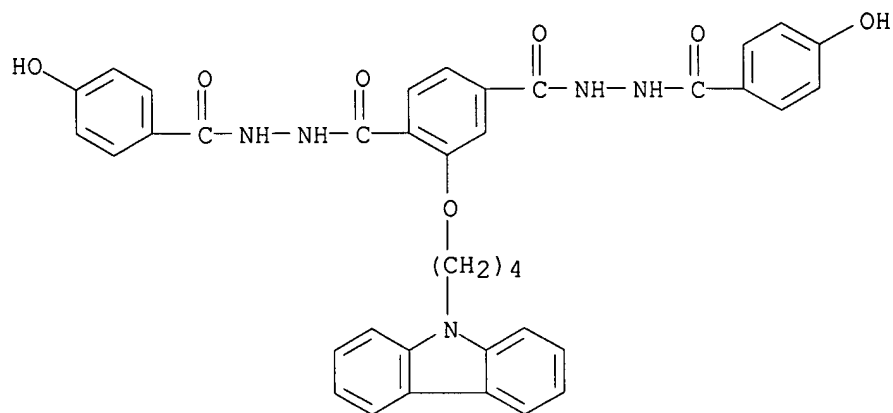
RN 881896-45-3 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[2-(9H-carbazol-9-yl)ethoxy]-,
bis[2-(4-hydroxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)



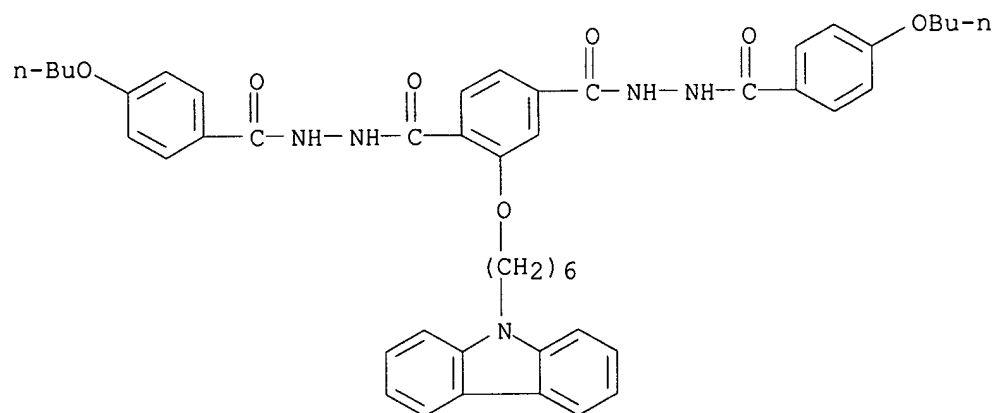
RN 881896-46-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-,
bis[2-(4-hydroxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)



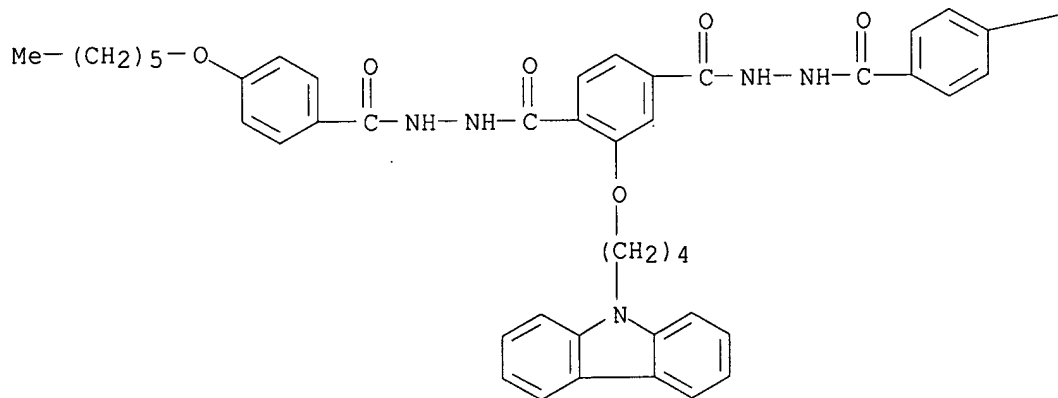
RN 881896-47-5 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[[6-(9H-carbazol-9-yl)hexyl]oxy]-, bis[2-(4-butoxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)



RN 881896-48-6 CAPLUS

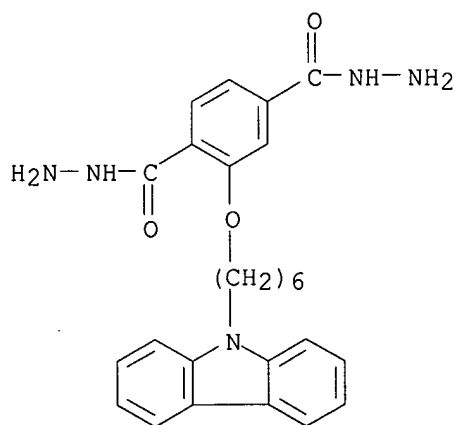
CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-, bis[2-[4-(hexyloxy)benzoyl]hydrazide] (9CI) (CA INDEX NAME)



PAGE 1-A

—O—(CH₂)₅—Me

IT 924881-57-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of electroluminescent mols. containing carbazole hole transport
 and oxadiazole electron transport units for a single-layer
 blue-emitting OLED)
 RN 924881-57-2 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-[[6-(9H-carbazol-9-yl)hexyl]oxy]-,
 1,4-dihydrazide (CA INDEX NAME)



RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2006:32921 CAPLUS
 DN 144:88556
 TI Preparation of tetramines for activation of binding of p53 to DNA
 IN Sato, Masakazu; Wada, Hisaya; Amada, Hideaki
 PA Taisho Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 36 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|------------------|------|----------|-----------------|----------|
| PI | JP 2006008533 | A | 20060112 | JP 2004-184095 | 20040622 |
| PRAI | JP 2004-184095 | | 20040622 | | |
| OS | MARPAT 144:88556 | | | | |

AB A[CONHCHZ(CH₂)_mZ]₂ [Z = CONH(CH₂)_nNR₁R₂; R₁, R₂ = H, C1-6 alkyl; R₁NR₂ may form saturated heterocyclyl; n = 1-5; m = 1, 2; A = substituted (cyclo)alkylene, naphthalenediyl, substituted xanthenediyl, etc.] or their medically acceptable salts, useful for induction of apoptosis in tumor cells, are prepared Thus, Z-Glu was amidated with Et₂N(CH₂)₃NH₂, deprotected, and refluxed with 2,4,5,6-tetrafluoroisophthaloyl dichloride to give tetramine, which at 100 μM showed 78.4% activation of binding of recombinant human p53 protein to DNA by Pab421 epitope peptide assay.

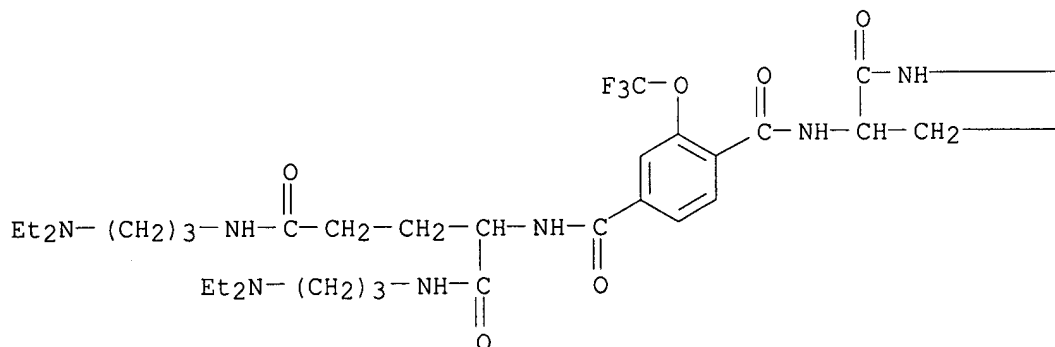
IT 872461-47-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetramines as antitumor agents)

RN 872461-47-7 CAPLUS
 CN 1,4-Benzenedicarboxamide, N,N'-bis[4-[[3-(diethylamino)propyl]amino]-1-
 [[3-(diethylamino)propyl]amino]carbonyl]-4-oxobutyl]-2-(trifluoromethoxy)-
 (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— (CH₂)₃—NEt₂

— CH₂—C(=O)—NH—(CH₂)₃—NEt₂

L3 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2005:1334801 CAPLUS
 DN 144:69830
 TI Preparation of 5-membered heterocycles as serine protease inhibitors for
 treatment of thromboembolic disorders.
 IN Hangeland, Jon J.; Quan, Mimi L.; Smallheer, Joanne M.; Bisacchi, Gregory
 S.; Corte, James R.; Friends, Todd J.; Sun, Zhong; Rossi, Karen A.;
 Cavallaro, Cullen L.
 PA USA
 SO U.S. Pat. Appl. Publ., 166 pp., which
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----|--|------|----------|-----------------|----------|
| PI | US 2005282805 | A1 | 20051222 | US 2005-151667 | 20050613 |
| | AU 2005254102 | A1 | 20051229 | AU 2005-254102 | 20050614 |
| | CA 2570472 | A1 | 20051229 | CA 2005-2570472 | 20050614 |
| | WO 2005123050 | A2 | 20051229 | WO 2005-US21212 | 20050614 |
| | WO 2005123050 | A3 | 20070104 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, | | | | |

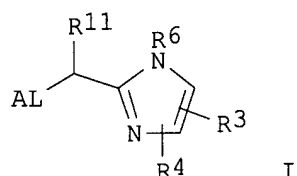
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

EP 1773786 A2 20070418 EP 2005-773261 20050614
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
HR, LV, MK, YU

CN 101006063 A 20070725 CN 2005-80027843 20050614
IN 2006DN07354 A 20070803 IN 2006-DN7354 20061206
KR 2007024601 A 20070302 KR 2006-726365 20061214
NO 2006005864 A 20070302 NO 2006-5864 20061215

PRAI US 2004-579638P P 20040615
US 2005-684127P P 20050524
US 2005-151667 A 20050613
WO 2005-US21212 W 20050614

OS MARPAT 144:69830
GI



AB Title compds. e.g. [I; A = (substituted) carbocyclyl, heterocyclyl; L = CONR10, CH2CONR10, SO2NR10, CH2CH2, CH2O, COCH2, etc.; R3 = (CH2)_rCONR8R9, (substituted) carbocyclyl(alkyl), heterocyclyl(alkyl), etc.; R4 = H, F, Cl, Br, iodo, OCF3, cyano, NO2, (substituted) alkyl, alkenyl, alkynyl, carbocyclyl, heterocyclyl, etc.; R6 = H; R8 = H, (substituted) alkyl, phenyl(alkyl), heterocyclylalkyl; R9 = H, (substituted) alkyl, phenyl(alkyl); R10 = H, (substituted) alkyl, alkenyl, alkynyl, carbocyclyl, heterocyclyl; r = 0-4], were prepared Thus, (S)-2-phenyl-1-(4-phenyl-1H-imidazol-2-yl)ethanamine bistrifluoroacetate (preparation given), 4-amidinobenzoic acid hydrochloride, and BOP reagent were stirred in pyridine for 16 h to give 3% (S)-4-carbamimidoyl-N-[2-phenyl-1-(4-phenyl-1H-imidazol-2-yl)ethyl]benzamide. I are useful as selective inhibitors of serine protease enzymes of the coagulation cascade and/or contact activation system such as thrombin, factor Xa, factor XIa, factor IXa, factor VIIa and/or plasma kallikrein; preferred I inhibited these with Ki values of ≤15 μM.

IT 872014-39-6P

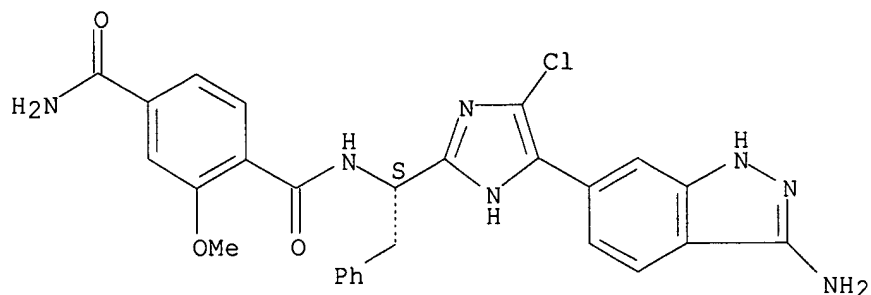
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of 5-membered heterocycles as serine protease inhibitors for treatment of thromboembolic disorders)

RN 872014-39-6 CAPLUS

CN 1,4-Benzenedicarboxamide, N1-[(1S)-1-[4-(3-amino-1H-indazol-6-yl)-5-chloro-1H-imidazol-2-yl]-2-phenylethyl]-2-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



IT 872016-44-9P

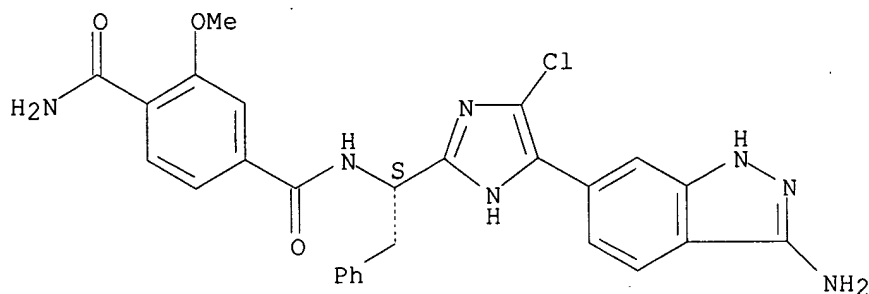
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 5-membered heterocycles as serine protease inhibitors for treatment of thromboembolic disorders)

RN 872016-44-9 CAPLUS

CN 1,4-Benzenedicarboxamide, N4-[(1S)-1-[4-(3-amino-1H-indazol-6-yl)-5-chloro-1H-imidazol-2-yl]-2-phenylethyl]-2-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:961964 CAPLUS

DN 143:248664

TI Preparation of terephthalamide peptidomimetic compounds for therapeutic use

IN Hamilton, Andrew D.; Yin, Hang

PA Yale University, USA

SO PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----|--|------|----------|-----------------|----------|
| PI | WO 2005079541 | A2 | 20050901 | WO 2005-US5557 | 20050222 |
| | WO 2005079541 | A3 | 20051103 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, | | | | |

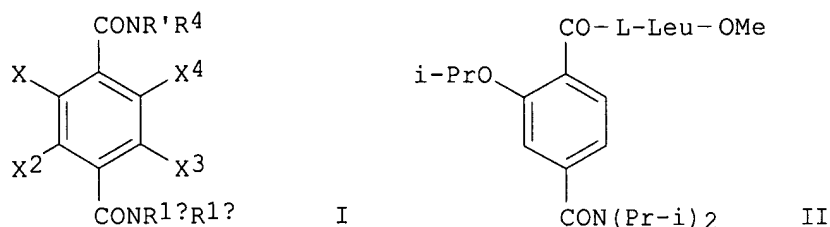
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

| | | | | |
|---------------|----|----------|-----------------|----------|
| AU 2005215051 | A1 | 20050901 | AU 2005-215051 | 20050222 |
| CA 2556447 | A1 | 20050901 | CA 2005-2556447 | 20050222 |
| EP 1723100 | A2 | 20061122 | EP 2005-713917 | 20050222 |

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
HR, LV, MK, YU

| | | | | |
|---------------|----|----------|----------------|----------|
| US 2007123592 | A1 | 20070531 | US 2006-588478 | 20061002 |
|---------------|----|----------|----------------|----------|

PRAI US 2004-546111P P 20040219
WO 2005-US5557 W 20050222
OS CASREACT 143:248664; MARPAT 143:248664
GI



AB The invention relates to compds. and pharmaceutical compns. based on terephthalamide which are proteomimetic and methods for inhibiting the interaction of an α -helical protein with another protein or binding site and for treating diseases or conditions which are modulated through these interactions. Compds. I [X is H, halo, R, OR, SR or an amino group, where R is H, (un)substituted alkyl, acyl, aryl, heteroaryl, alkylenearyl or alkyleneheteroaryl; X2, X3, X4 are independently H, halo, OH, Rc, ORc, where Rc is (un)substituted alkyl, acyl, aryl or alkylenearyl; R4 is H, (un)substituted alkyl, alkenyl or alkylene amine; R', R1a, R1b are any group given for R4 or (CH2)0-2CHR2CO2H or an alkyl ester, where R2 is independently H or (un)substituted hydrocarbon, alkoxy, ester, alkanol, alkanolic acid, amine, etc.; or N-R' or NR1aR1b form an amino acid residue] are claimed. Thus, peptidomimetic compound II, prepared via coupling reaction of L-leucine Me ester hydrochloride, showed inhibitory constant $K_i = 0.781 \pm 0.070 \mu\text{M}$ in a fluorescence polarization assay (binding affinity for Bcl-XL).

IT 681466-00-2P

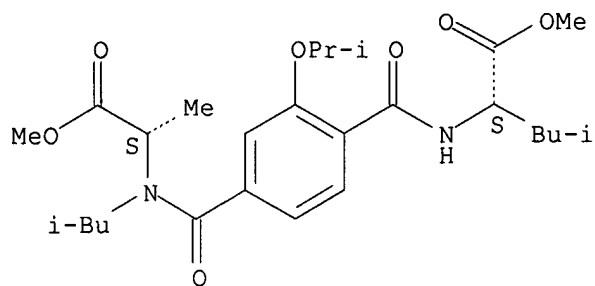
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(conformation; preparation of terephthalamide peptidomimetic compds. for therapeutic use)

RN 681466-00-2 CAPLUS

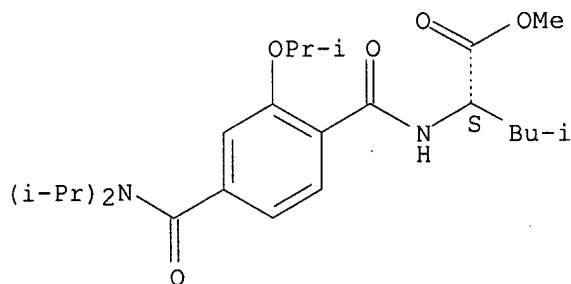
CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



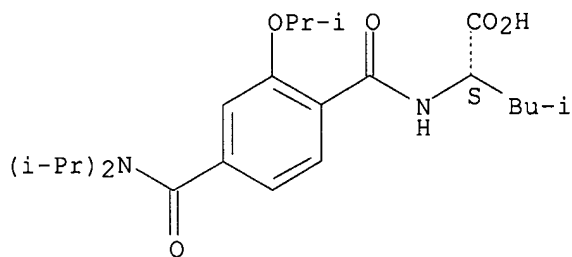
IT 681465-54-3P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of terephthalamide peptidomimetic compds. for therapeutic use)
 RN 681465-54-3 CAPLUS
 CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-60-1P 681465-62-3P
 681465-68-9P 681465-70-3P 681465-74-7P
 852065-21-5P 852065-22-6P 852065-26-0P
 852065-27-1P 852065-28-2P 852065-29-3P
 852065-30-6P 852065-31-7P 852065-32-8P
 852065-33-9P 852065-34-0P 852065-35-1P
 852065-36-2P 852065-37-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of terephthalamide peptidomimetic compds. for therapeutic use)
 RN 681465-56-5 CAPLUS
 CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

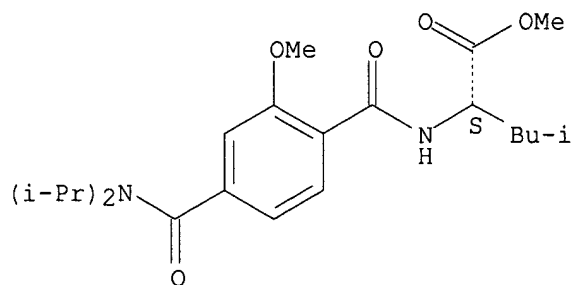
Absolute stereochemistry.



RN 681465-60-1 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

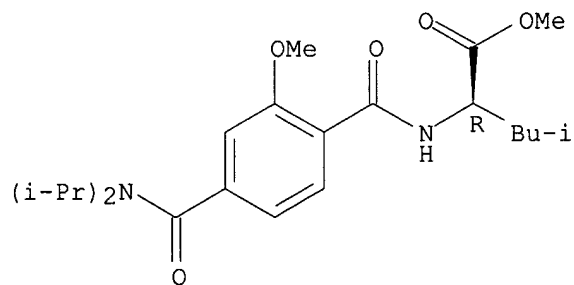
Absolute stereochemistry. Rotation (-).



RN 681465-62-3 CAPLUS

CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

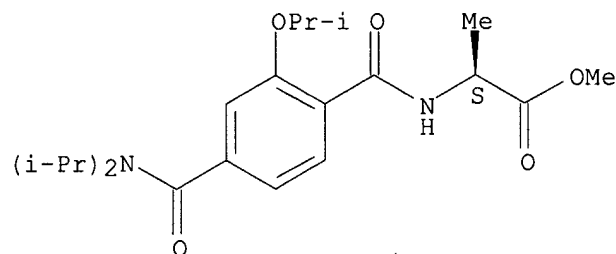
Absolute stereochemistry.



RN 681465-68-9 CAPLUS

CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

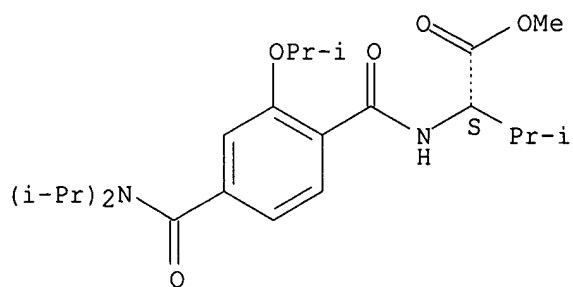
Absolute stereochemistry.



RN 681465-70-3 CAPLUS

CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

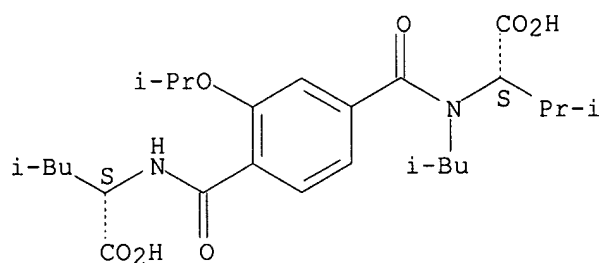
Absolute stereochemistry.



RN 681465-74-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

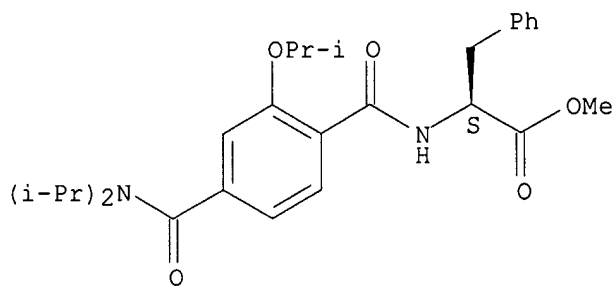
Absolute stereochemistry.



RN 852065-21-5 CAPLUS

CN L-Phenylalanine, N-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

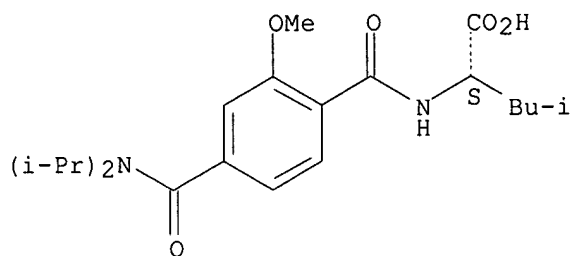
Absolute stereochemistry.



RN 852065-22-6 CAPLUS

CN L-Leucine, N-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]- (CA INDEX NAME)

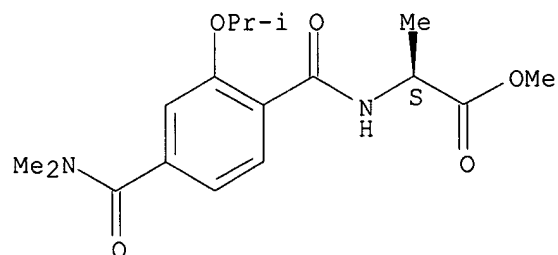
Absolute stereochemistry.



RN 852065-26-0 CAPLUS

CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

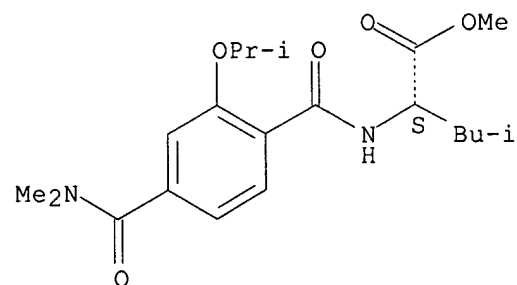
Absolute stereochemistry. Rotation (+).



RN 852065-27-1 CAPLUS

CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

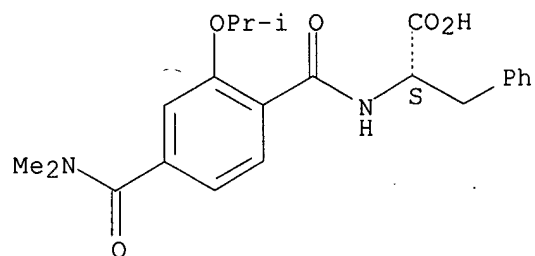
Absolute stereochemistry.



RN 852065-28-2 CAPLUS

CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
(CA INDEX NAME)

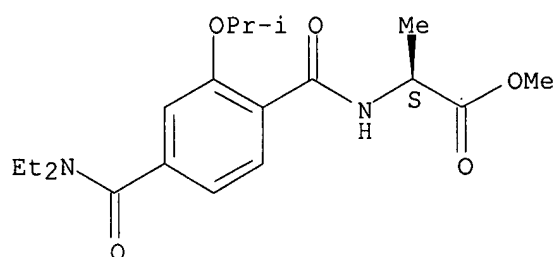
Absolute stereochemistry. Rotation (+).



RN 852065-29-3 CAPLUS

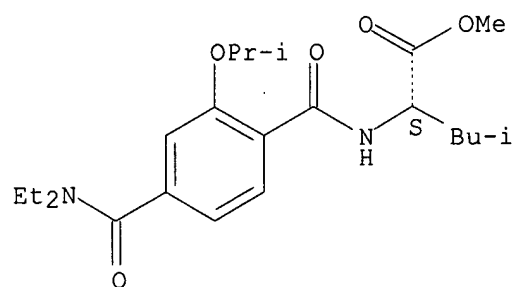
CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



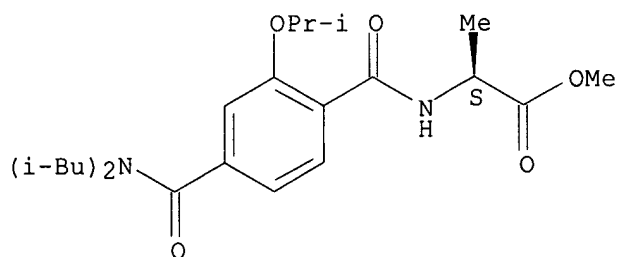
RN 852065-30-6 CAPLUS
 CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
 methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



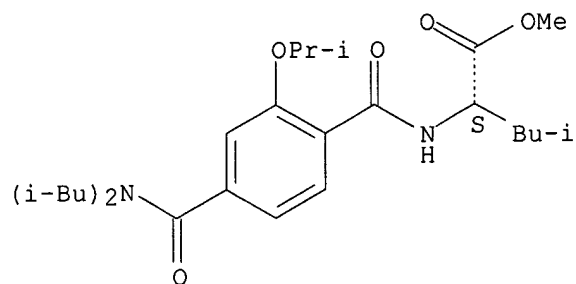
RN 852065-31-7 CAPLUS
 CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-
 methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



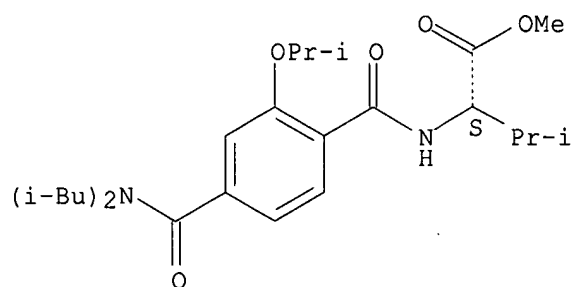
RN 852065-32-8 CAPLUS
 CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-
 methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



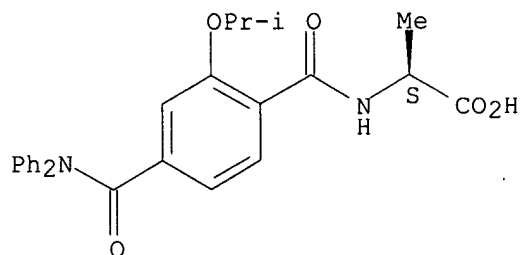
RN 852065-33-9 CAPLUS
CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



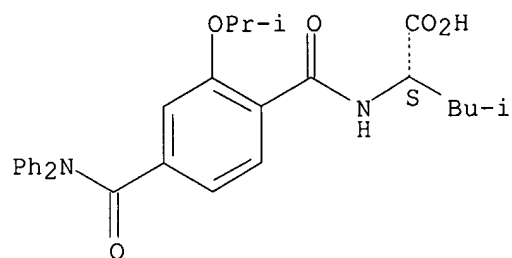
RN 852065-34-0 CAPLUS
CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



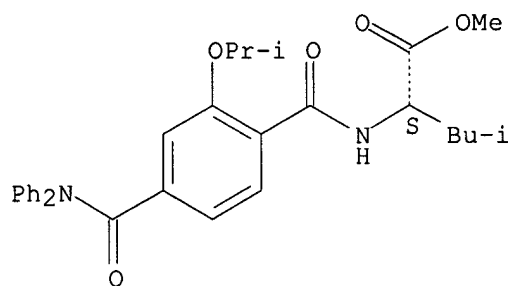
RN 852065-35-1 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

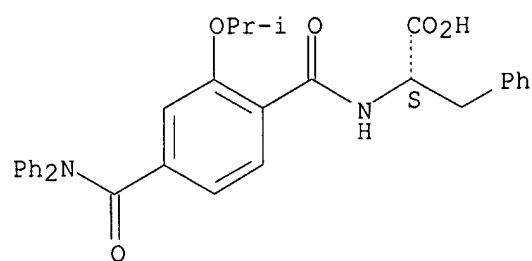
Absolute stereochemistry. Rotation (-).



RN 852065-37-3 CAPLUS

CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L3 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:312873 CAPLUS

DN 143:39922

TI Structural Requirements for Factor Xa Inhibition by 3-Oxybenzamides with
Neutral P1 Substituents: Combining X-ray Crystallography, 3D-QSAR, and
Tailored Scoring Functions

AU Matter, Hans; Will, David W.; Nazare, Marc; Schreuder, Herman; Laux,
Volker; Wehner, Volkmar

CS DIA Chemistry, Aventis Pharma Deutschland GmbH, Frankfurt am Main,
D-65926, Germany

SO Journal of Medicinal Chemistry (2005), 48(9), 3290-3312

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB The design, synthesis, and structure-activity relationship of
3-oxybenzamides as potent inhibitors of the coagulation protease factor Xa
are described on the basis of X-ray structures, privileged structure
motifs, and SAR information. A total of six x-ray structures of
fXa/inhibitor complexes led us to identify the major protein-ligand
interactions. The binding mode is characterized by a lipophilic
dichlorophenyl substituent interacting with Tyr228 in the protease S1
pocket, while polar parts are accommodated in S4. This alignment in
combination with docking allowed derivation of 3D-QSAR models and tailored
scoring functions to rationalize biol. affinity and provide guidelines for
optimization. The resulting models showed good correlation coeffs. and
predictions of external test sets. Furthermore, they correspond to
binding site topologies in terms of steric, electrostatic, and hydrophobic
complementarity. Two approaches to derive tailored scoring functions
combining binding site and ligand information led to predictive models
with acceptable predictions of the external set. Good correlations to
exptl. affinities were obtained for both AFMoC (adaptation of fields for
mol. comparison) and the novel TScore function. The SAR information from
3D-QSAR and tailored scoring functions agrees with all exptl. data and

provides guidelines and reasonable activity estns. for novel fXa inhibitors.

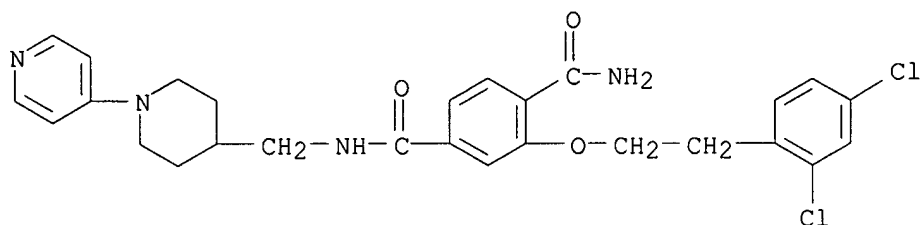
IT 717902-18-6

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(structural requirements for factor Xa inhibition by 3-oxybenzamides with neutral P1 substituents)

RN 717902-18-6 CAPLUS

CN 1,4-Benzenedicarboxamide, 2-[2-(2,4-dichlorophenyl)ethoxy]-N4-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)



RE.CNT 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:267006 CAPLUS

DN 142:482288

TI Terephthalamide Derivatives as Mimetics of Helical Peptides: Disruption of the Bcl-xL/Bak Interaction

AU Yin, Hang; Lee, Gui-in; Sedey, Kristine A.; Rodriguez, Johanna M.; Wang, Hong-Gang; Sebt, Said M.; Hamilton, Andrew D.

CS Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA

SO Journal of the American Chemical Society (2005), 127(15), 5463-5468

CODEN: JACSAT; ISSN: 0002-7863

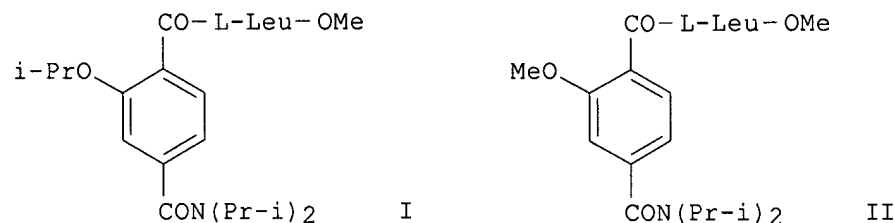
PB American Chemical Society

DT Journal

LA English

OS CASREACT 142:482288

GI



AB A series of Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, was designed to mimic the α -helical region of the Bak peptide. These mols. showed favorable in-vitro activities in disrupting the Bcl-xL/Bak BH3 domain complex (terephthalamides I and II, $K_i = 0.78 \pm 0.07$ and $1.85 \pm 0.32 \mu\text{M}$, resp.). Extensive structure-affinity studies demonstrated a correlation between the ability of terephthalamide derivs. to disrupt Bcl-xL/Bak complex formation and the size of variable side chains on these mols. Treatment of human HEK293 cells with the terephthalamide derivative 26 resulted in disruption of the Bcl-xL/Bax interaction in whole cells with an IC_{50} of $35.0 \mu\text{M}$. Computational docking simulations and NMR expts. suggested that the binding cleft for

the BH3 domain of the Bak peptide on the surface of Bcl-xL is the target area for these synthetic inhibitors.

IT 681465-54-3P

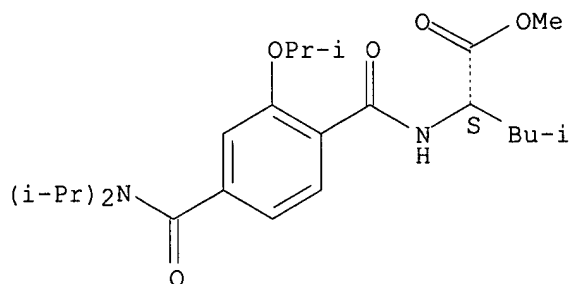
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-54-3 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-58-7P 681465-60-1P

681465-62-3P 681465-68-9P 681465-70-3P

681465-74-7P 852065-21-5P 852065-22-6P

852065-26-0P 852065-27-1P 852065-28-2P

852065-29-3P 852065-30-6P 852065-31-7P

852065-32-8P 852065-33-9P 852065-34-0P

852065-35-1P 852065-36-2P 852065-37-3P

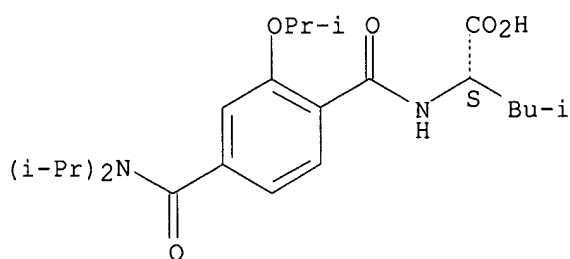
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-56-5 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

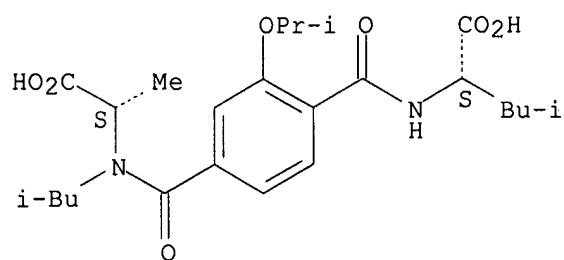
Absolute stereochemistry.



RN 681465-58-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

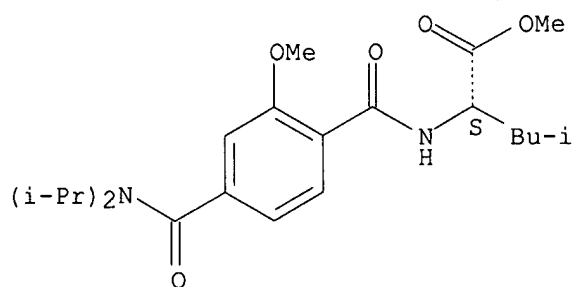
Absolute stereochemistry. Rotation (-).



RN 681465-60-1 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

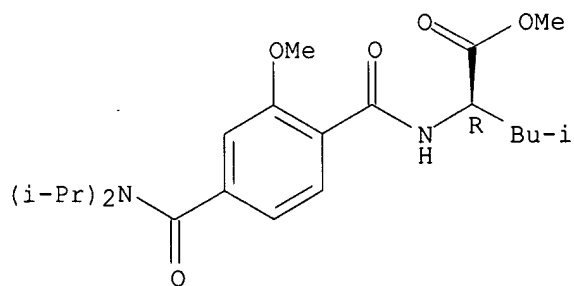
Absolute stereochemistry. Rotation (-).



RN 681465-62-3 CAPLUS

CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

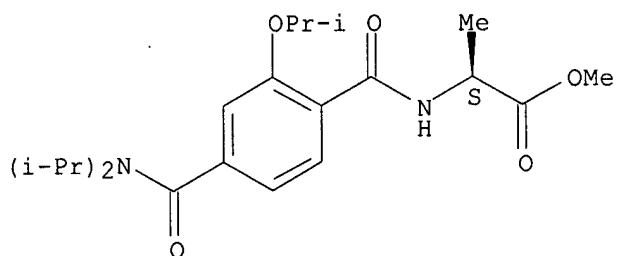
Absolute stereochemistry.



RN 681465-68-9 CAPLUS

CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

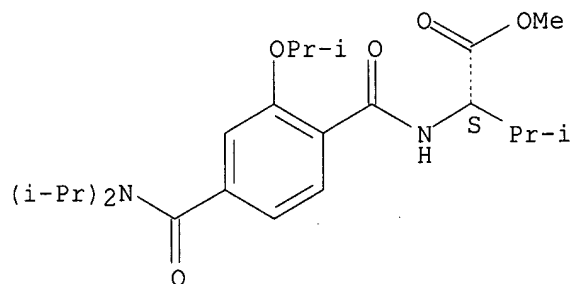
Absolute stereochemistry.



RN 681465-70-3 CAPLUS

CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

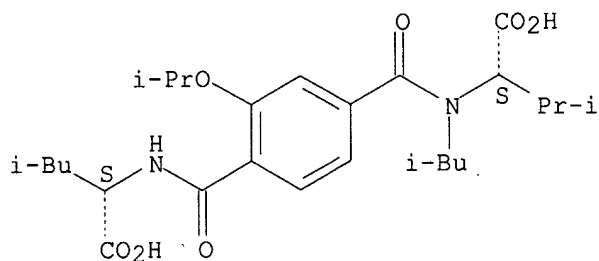
Absolute stereochemistry.



RN 681465-74-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

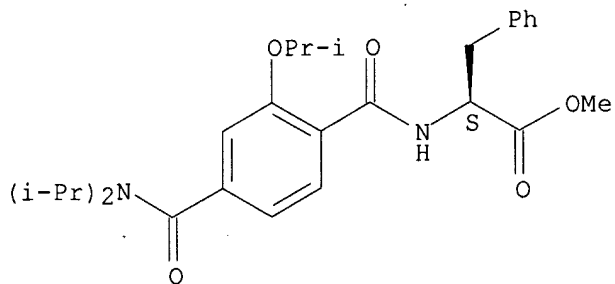
Absolute stereochemistry.



RN 852065-21-5 CAPLUS

CN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

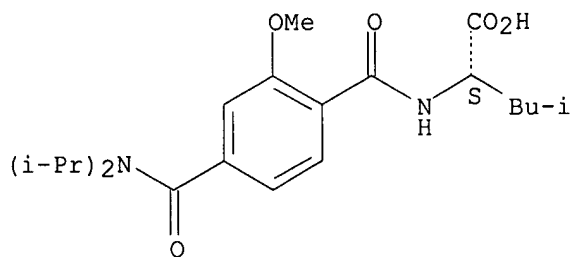
Absolute stereochemistry.



RN 852065-22-6 CAPLUS

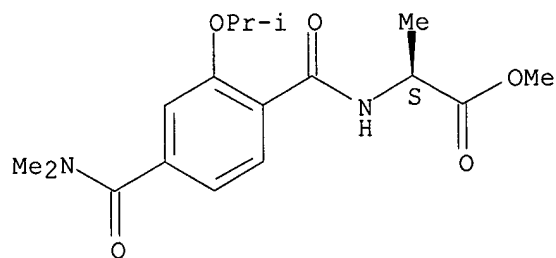
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



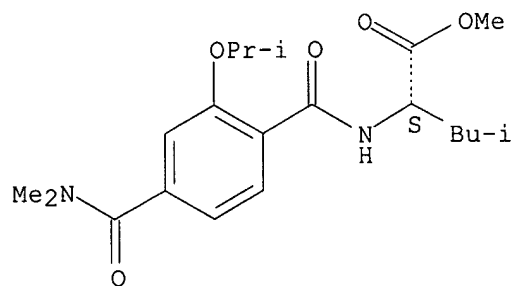
RN 852065-26-0 CAPLUS
 CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
 methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



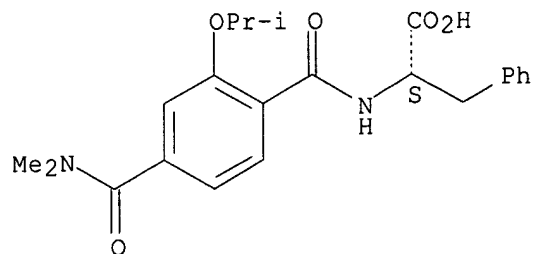
RN 852065-27-1 CAPLUS
 CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
 methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 852065-28-2 CAPLUS
 CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
 (CA INDEX NAME)

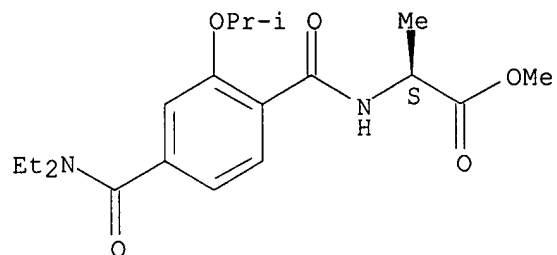
Absolute stereochemistry. Rotation (+).



RN 852065-29-3 CAPLUS

CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

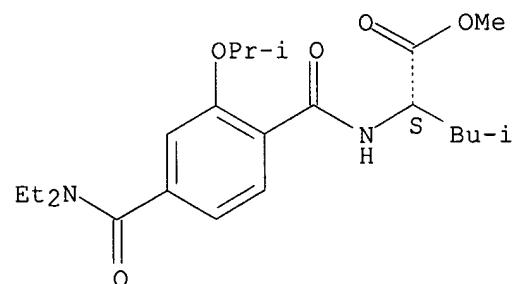
Absolute stereochemistry. Rotation (+).



RN 852065-30-6 CAPLUS

CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

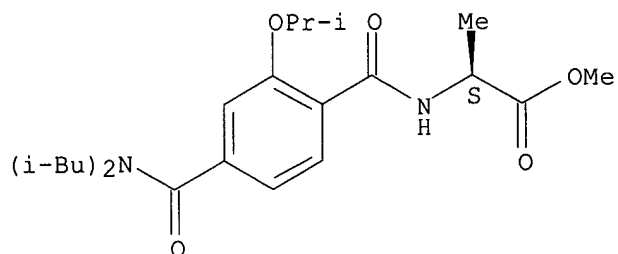
Absolute stereochemistry. Rotation (+).



RN 852065-31-7 CAPLUS

CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-
methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

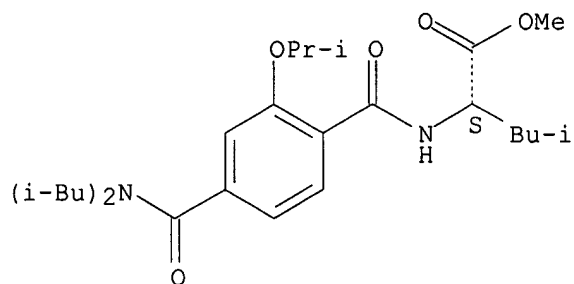
Absolute stereochemistry. Rotation (+).



RN 852065-32-8 CAPLUS

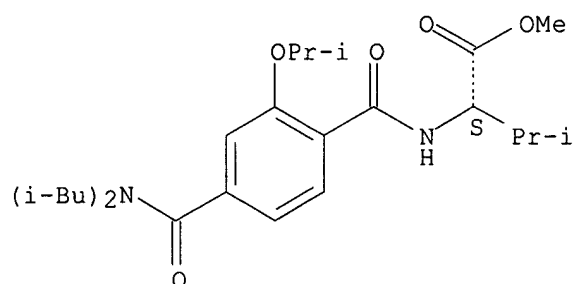
CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-
methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



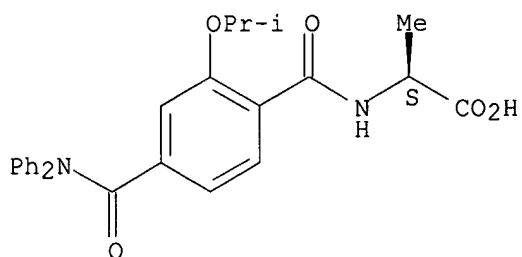
RN 852065-33-9 CAPLUS
 CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



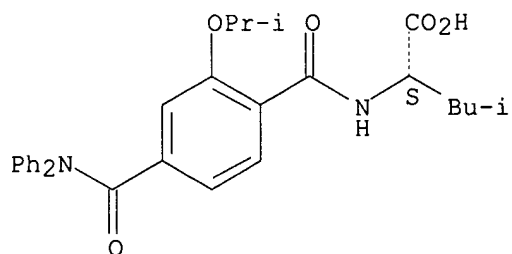
RN 852065-34-0 CAPLUS
 CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



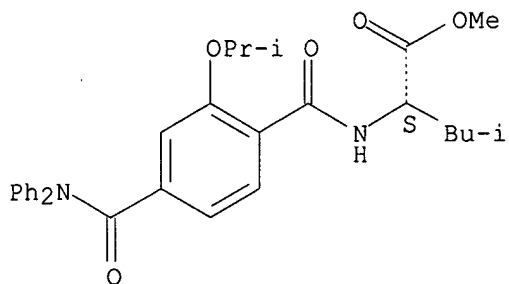
RN 852065-35-1 CAPLUS
 CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



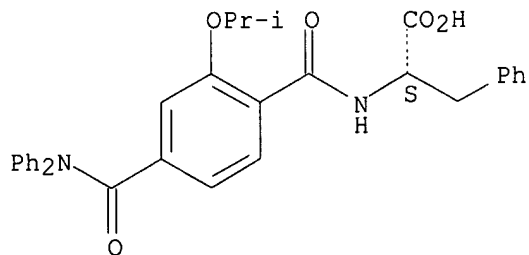
RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



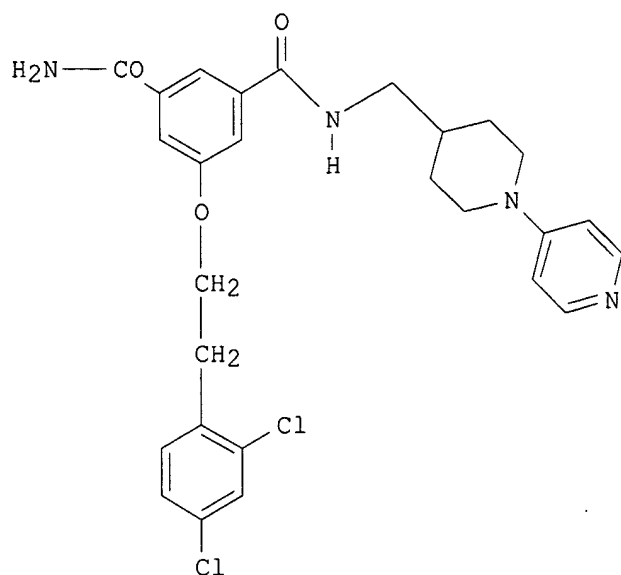
RN 852065-37-3 CAPLUS
CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:362563 CAPLUS
DN 141:98999
TI Novel factor Xa inhibitors based on a benzoic acid scaffold and
incorporating a neutral P1 ligand
AU Nazare, Marc; Matter, Hans; Klingler, Otmar; Al-Obeidi, Fahad; Schreuder,
Herman; Zoller, Gerhard; Czech, Jorg; Lorenz, Martin; Dudda, Angela;
Peyman, Anusch; Nestler, Hans Peter; Urmann, Matthias; Bauer, Armin; Laux,
Volker; Wehner, Volkmar; Will, David W.
CS Aventis Pharma Deutschland GmbH, Frankfurt, D-65926, Germany
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2801-2805
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 141:98999
GI



I

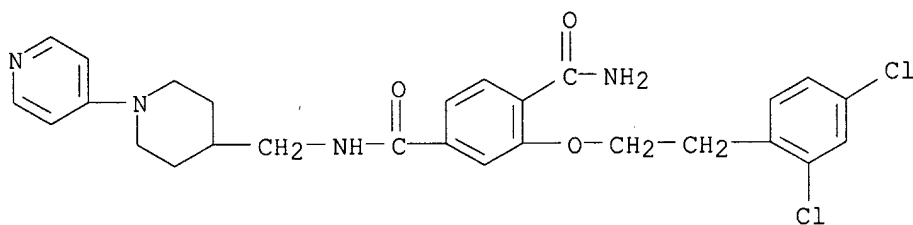
AB A series of novel, highly potent, achiral factor Xa inhibitors based on a benzoic acid scaffold and containing a chlorophenethyl moiety directed towards the protease S1 pocket is described. A number of structural features, such as the requirements of the P1, P4 and ester-binding pocket ligands were explored with respect to inhibition of factor Xa. Compound (I) was the most potent compound in a series of antithrombotic secondary assays.

IT 717902-18-6

RL: PAC (Pharmacological activity); BIOL (Biological study)
(novel factor Xa inhibitors based on a benzoic acid scaffold and incorporating a neutral P1 ligand)

RN 717902-18-6 CAPLUS

CN 1,4-Benzenedicarboxamide, 2-[2-(2,4-dichlorophenyl)ethoxy]-N4-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:189140 CAPLUS

DN 140:350050

TI Terephthalamide derivatives as mimetics of the helical region of Bak peptide target Bcl-xL protein

AU Yin, Hang; Hamilton, Andrew D.

CS Department of Chemistry, Yale University, New Haven, CT, 06511, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(6), 1375-1379

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

OS CASREACT 140:350050

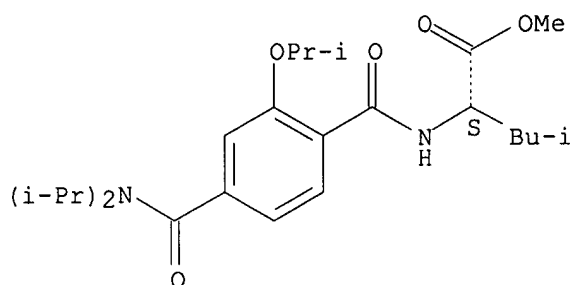
AB A group of novel Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, were designed to mimic the α -helical region of the Bak peptide. Good in vitro inhibition potencies in disrupting the Bak/Bcl-xL complex have been observed (terephthalamide 4, $K_i=0.78\pm0.07$ μ M).

IT 681465-54-3P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-54-3 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

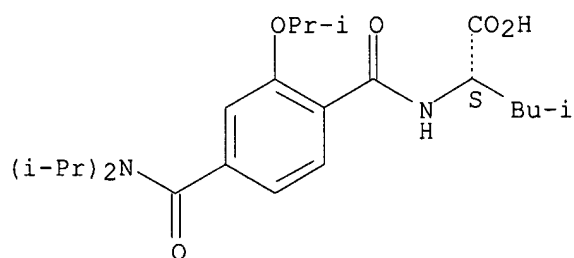


IT 681465-56-5P 681465-58-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-56-5 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

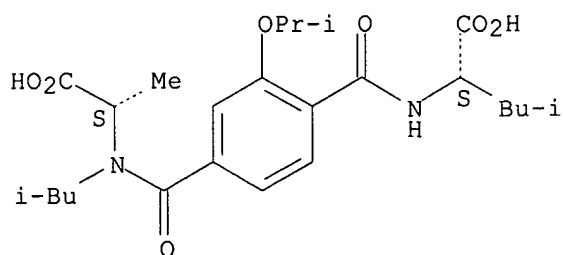
Absolute stereochemistry.



RN 681465-58-7 CAPLUS

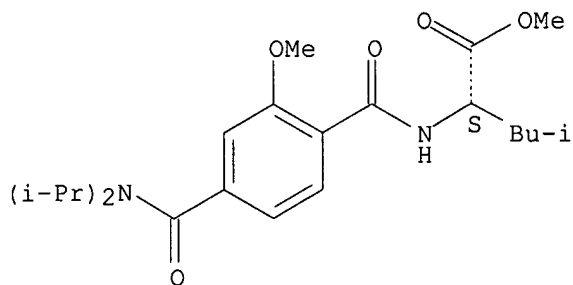
CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



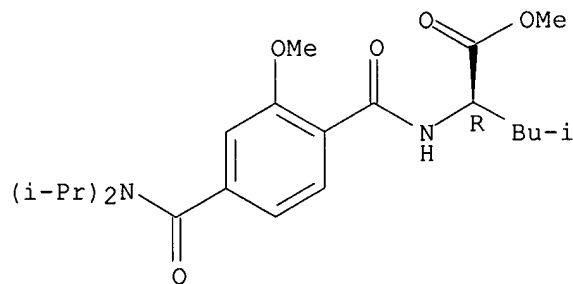
IT 681465-60-1 681465-62-3 681465-68-9
 681465-70-3 681465-72-5 681465-74-7
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (terephthalamide derivs. as novel Bcl-xL/Bak antagonists)
 RN 681465-60-1 CAPLUS
 CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-,
 methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



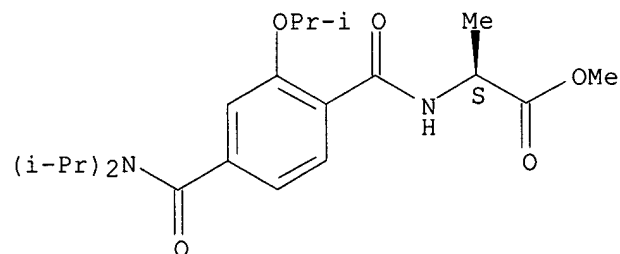
RN 681465-62-3 CAPLUS
 CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-,
 methyl ester (CA INDEX NAME)

Absolute stereochemistry.



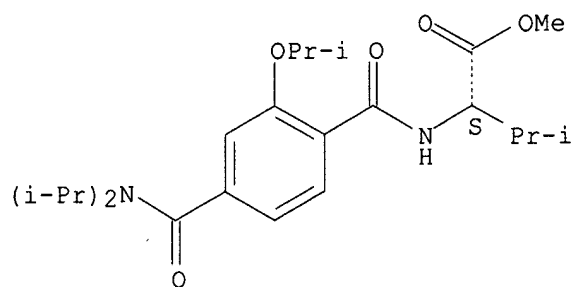
RN 681465-68-9 CAPLUS
 CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-
 methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 681465-70-3 CAPLUS
 CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-
 methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

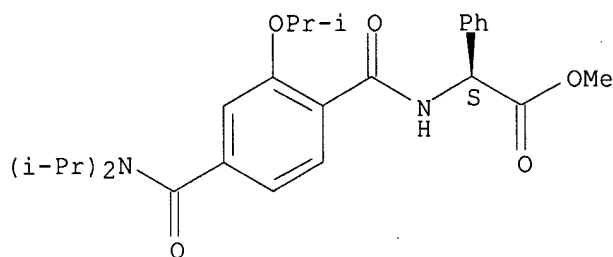
Absolute stereochemistry.



RN 681465-72-5 CAPLUS

CN Benzeneacetic acid, α-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

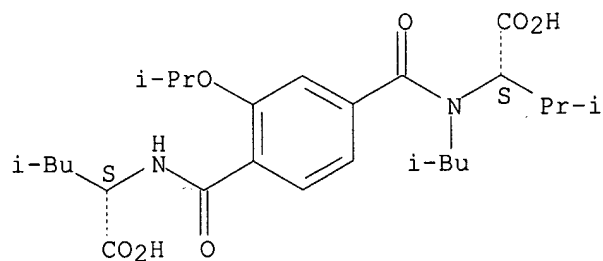
Absolute stereochemistry.



RN 681465-74-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



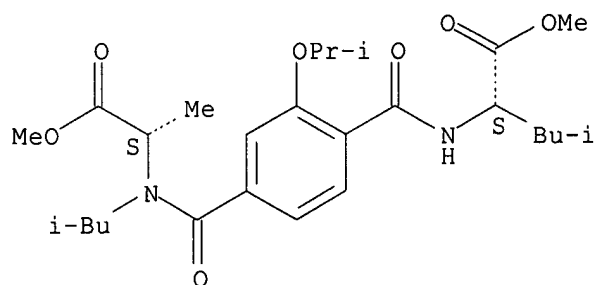
IT 681466-00-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681466-00-2 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:991333 CAPLUS
DN 140:35967
TI Methods of treating Alzheimers disease using aromatically substituted
ω-amino-alkanoic acid amides and alkanolic acid diamides
IN Maillard, Michel; Varghese, John
PA Elan Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2003103652 | A1 | 20031218 | WO 2003-US18283 | 20030611 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003237546 | A1 | 20031222 | AU 2003-237546 | 20030611 |
| US 2006089355 | A1 | 20060427 | US 2005-517981 | 20050714 |
| PRAI US 2002-387756P | P | 20020611 | | |
| WO 2003-US18283 | W | 20030611 | | |

OS MARPAT 140:35967

AB Disclosed are methods for treating Alzheimer's disease (no data), and other diseases (no data), and/or inhibiting beta-secretase enzyme (no data), and/or inhibiting deposition of amyloid β peptide (no data) in a mammal, using ω-amino-alkanoic acid amides and alkanolic acid diamides (R1-X1-NH-X2-CH(R2)CH2CH(R3)CH(OH)CH2CH(R4)C(O)NH-R5 (I); variables defined below; e.g. (2S,4S,5S,7R)-N-(4-amino-7-butyl-7-carbamoyl-5-hydroxy-2-isopropyloctyl)-3-methoxy-2-(3-methoxypropoxy)benzamide). Many example preps. are included but all of them comprise an English translation of a German patent (EP 0716077 A1; 1996; CA file accession number 125:167576). For I: R1 is a 2-RA-3-RB-Ph radical, a 2-RA-4-Rc-Ph radical, a 2-RA-pyridin-3-yl radical a 3-RA-pyridin-2-yl radical or a 1-RD-indol-3-yl radical, wherein one of the radicals RA and RB is an aliphatic or heterocycloaliph.-aliphatic radical or free or aliphatically, araliphatically or heteroaraliphatically etherified hydroxy and the other is H, an aliphatic radical or free or esterified or amidated carboxy, RC is H, an aliphatic radical, free or aliphatically, araliphatically, heteroaraliphatically or heteroarylaliphatically etherified hydroxy or an unsubstituted or heteroaliphatically substituted amino group, and RD is an aliphatic, araliph. or heteroaliph. radical, one of the radicals X1 and X2 is

carbonyl and the other is methylene, R2 is an aliphatic radical, R3 is unsubstituted or aliphatically substituted amino, R4 is an aliphatic or araliph. radical, and R5 is an aliphatic or cycloaliph.-aliphatic radical or an optionally hydrogenated and/or oxo-substituted heteroaryl radical or an optionally hydrogenated and/or oxo-substituted heteroaryl or heteroaliph. radical bonded via a C atom.

IT 179995-21-2P 179995-22-3P 179995-71-2P
179995-72-3P 179995-73-4P 179995-74-5P
179995-97-2P 179996-13-5P 180183-42-0P
180183-63-5P

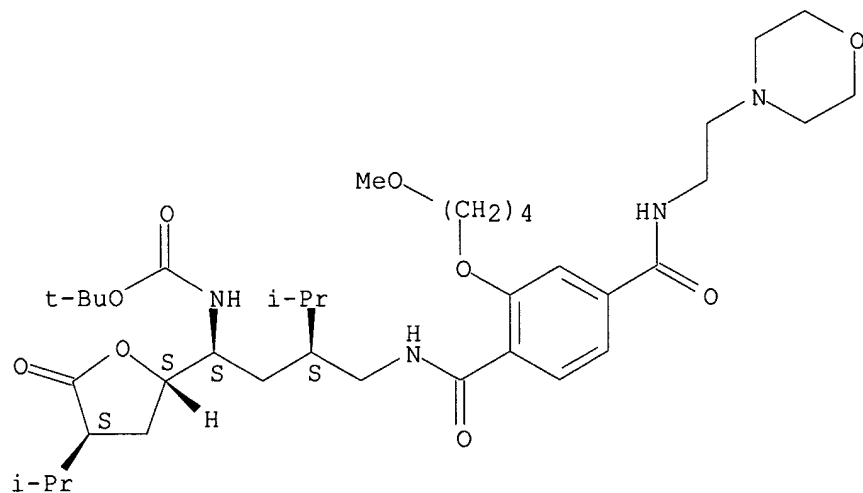
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; methods of treating Alzheimers disease using aromatically substituted ω -amino-alkanoic acid amides and alkanolic acid diamides)

RN 179995-21-2 CAPLUS

CN Carbamic acid, [(1S,3S)-3-[[[2-(4-methoxybutoxy)-4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]benzoyl]amino]methyl]-4-methyl-1-[(2S,4S)-tetrahydro-4-(1-methylethyl)-5-oxo-2-furanyl]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

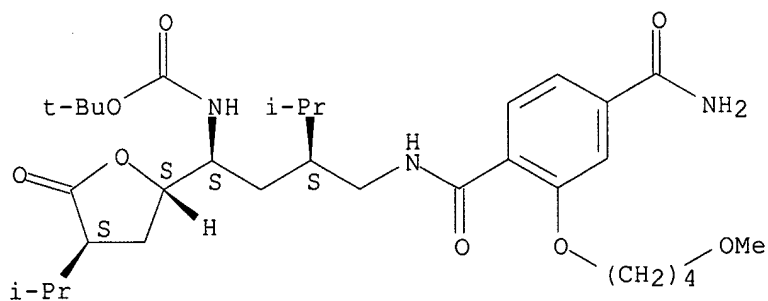
Absolute stereochemistry.



RN 179995-22-3 CAPLUS

CN Carbamic acid, [(1S,3S)-3-[[[4-(aminocarbonyl)-2-(4-methoxybutoxy)benzoyl]amino]methyl]-4-methyl-1-[(2S,4S)-tetrahydro-4-(1-methylethyl)-5-oxo-2-furanyl]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

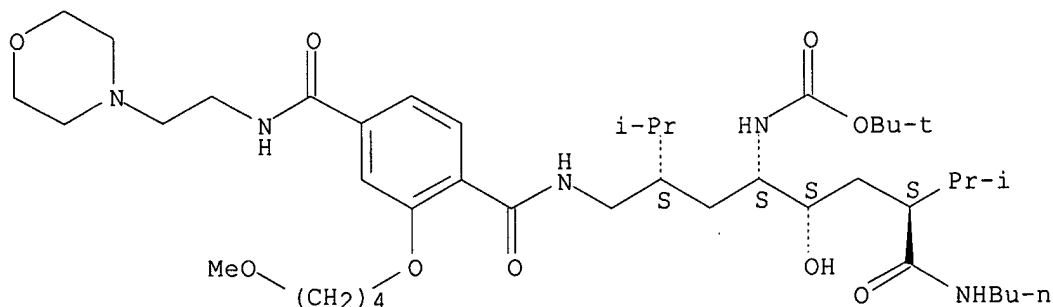
Absolute stereochemistry.



RN 179995-71-2 CAPLUS

CN Carbamic acid, [(1S,2S,4S)-4-[(butylamino)carbonyl]-2-hydroxy-1-[(2S)-2-[[[2-(4-methoxybutoxy)-4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]benzoyl]amino]methyl]-3-methylbutyl]-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

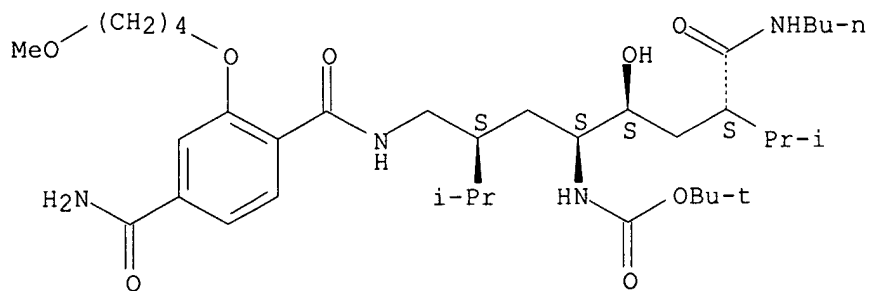
Absolute stereochemistry.



RN 179995-72-3 CAPLUS

CN Carbamic acid, [(1S,2S,4S)-1-[(2S)-2-[[[4-(aminocarbonyl)-2-(4-methoxybutoxy)benzoyl]amino]methyl]-3-methylbutyl]-4-[(butylamino)carbonyl]-2-hydroxy-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

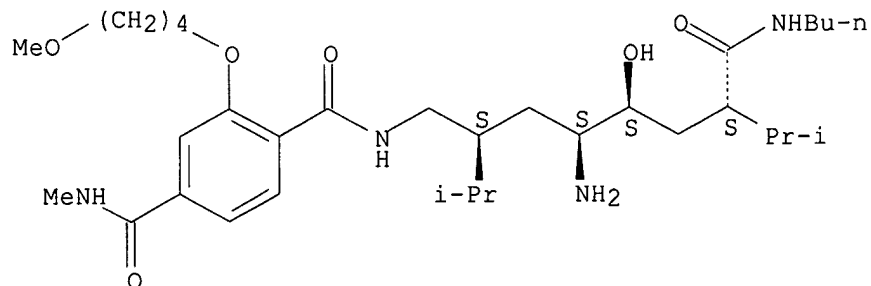
Absolute stereochemistry.



RN 179995-73-4 CAPLUS

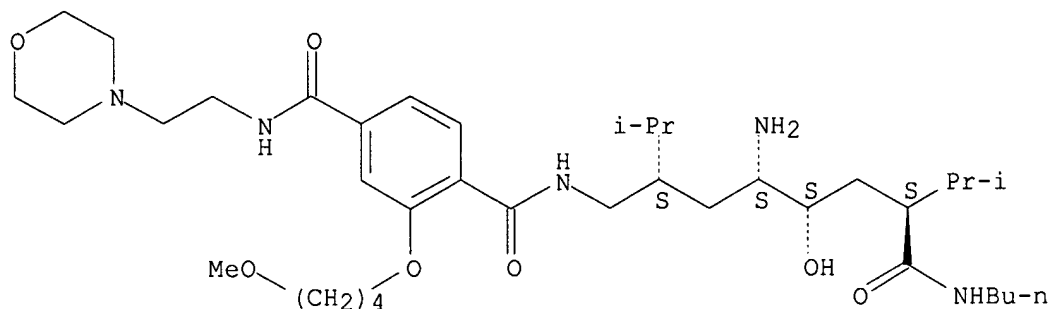
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-N4-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 179995-74-5 CAPLUS
 CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-
 [(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-
 methoxybutoxy)-N4-[2-(4-morpholinyl)ethyl]-, monohydrochloride (9CI) (CA
 INDEX NAME)

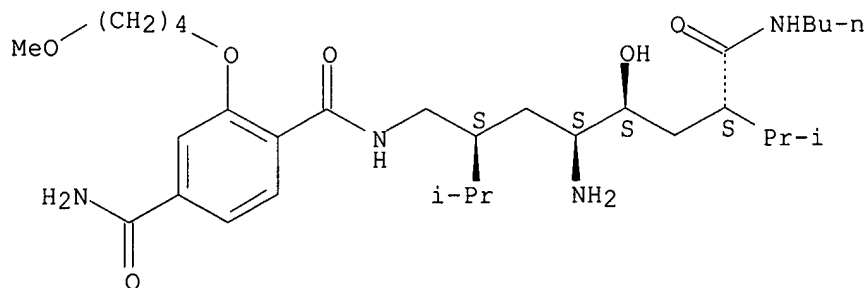
Absolute stereochemistry.



● HCl

RN 179995-97-2 CAPLUS
 CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-
 [(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-
 methoxybutoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

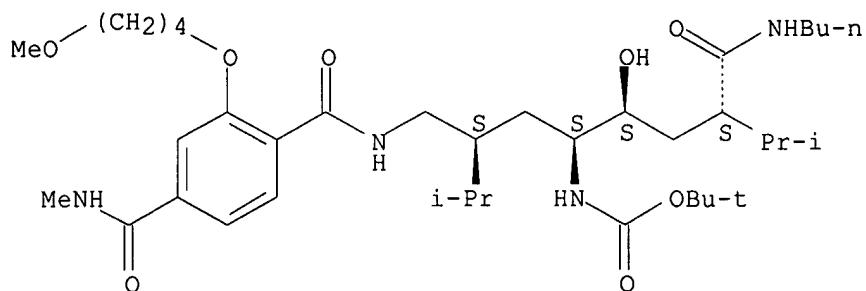
Absolute stereochemistry.



● HCl

RN 179996-13-5 CAPLUS
 CN Carbamic acid, [(1S,2S,4S)-4-[(butylamino)carbonyl]-2-hydroxy-1-[(2S)-2-
 [[2-(4-methoxybutoxy)-4-[(methylamino)carbonyl]benzoyl]amino]methyl]-3-
 methylbutyl]-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX
 NAME)

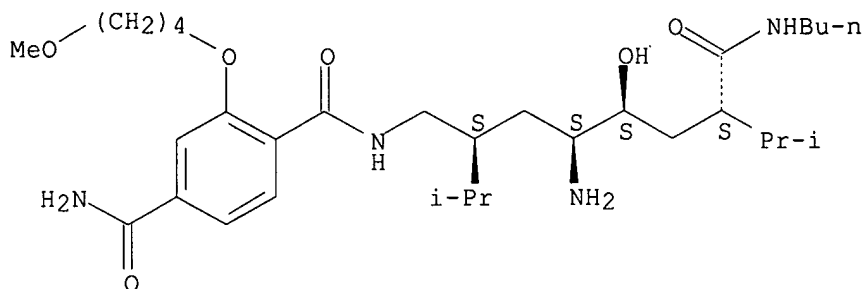
Absolute stereochemistry.



RN 180183-42-0 CAPLUS

CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)- (CA INDEX NAME)

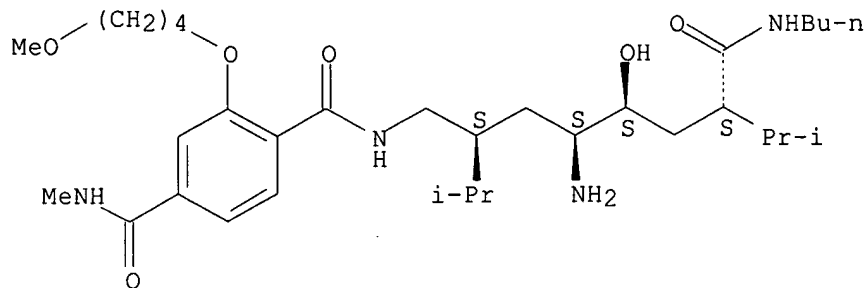
Absolute stereochemistry.



RN 180183-63-5 CAPLUS

CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-N4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:952818 CAPLUS
DN 140:146599
TI Unsaturated alkoxy-substituted poly(p-phenylene 1,3,4-oxadiazole)s:
Synthesis and chemical-physical characterization
AU Capitani, Donatella; Laurienzo, Paola; Malinconico, Mario; Proietti,
Noemi; Roviello, Antonio
CS Istituto di Metodologie Chimiche, C.N.R., Monterotondo Stazione, 00016,
Italy
SO Journal of Polymer Science, Part A: Polymer Chemistry (2003), 41(24),
3916-3928

CODEN: JPACEC; ISSN: 0887-624X

PB John Wiley & Sons, Inc.

DT Journal

LA English

AB A new series of alkoxy-substituted poly(p-phenylene 1,3,4-oxadiazole)s modified by the insertion of small percentages of various comonomers were synthesized through the precursor polyhydrazides. The comonomers used contained trans double bonds or meta-alkoxy-substituted aromatic rings to improve the solubility of the final polymers. The synthesized copolymers were chemical characterized by ^1H NMR and Fourier transform IR spectroscopy. In some cases, the copolymers really showed improved solubility in organic solvents.

The ^{15}N solid-state NMR technique was applied to examine the degree of conversion from the precursor polyhydrazides to the final polymers, which determined the effective conjugated length in the target polyoxadiazoles. Thermal stability and structural characteristics of all the polymers as well as a preliminary investigation on the optical properties of polyoxadiazoles are also reported. The copolymers retained high absorbance in the UV region and high transmission in the whole telecommunication range.

IT 428516-44-3P 651054-59-0P 651054-60-3P
651054-61-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(precursor; synthesis and chemical-phys. characterization of unsatd. alkoxy-substituted poly(phenylene oxadiazole)s)

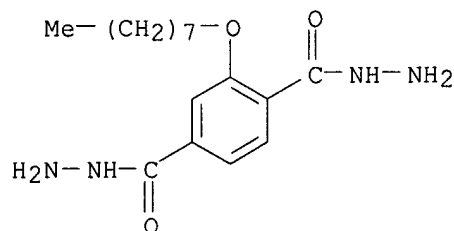
RN 428516-44-3 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-40-9

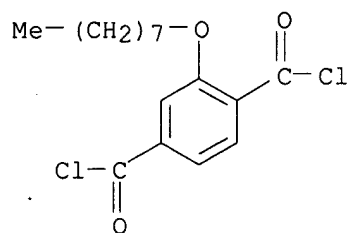
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

CMF C16 H20 Cl2 O3



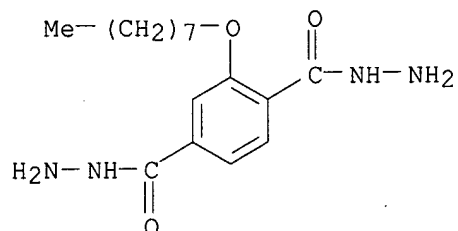
RN 651054-59-0 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-40-9

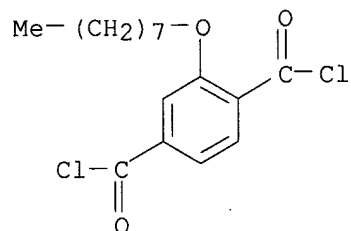
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

CMF C16 H20 Cl2 O3

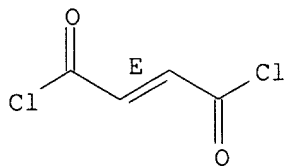


CM 3

CRN 627-63-4

CMF C4 H2 Cl2 O2

Double bond geometry as shown.



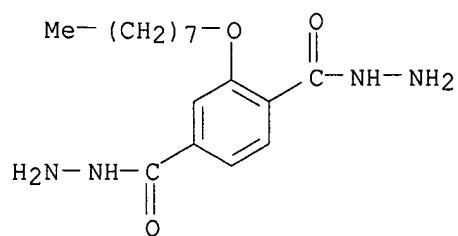
RN 651054-60-3 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-40-9

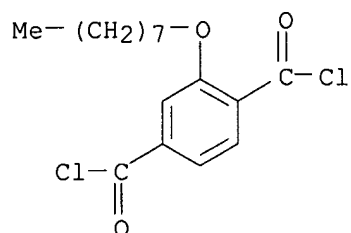
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

CMF C16 H20 Cl2 O3

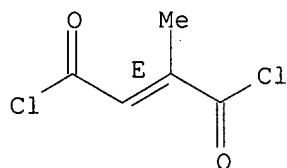


CM 3

CRN 20537-97-7

CMF C5 H4 Cl2 O2

Double bond geometry as shown.



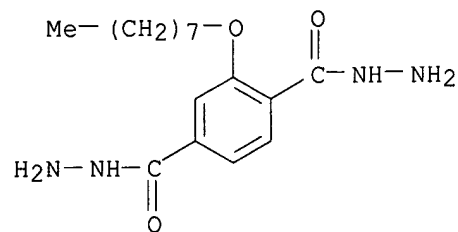
RN 651054-61-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride, 2-(octyloxy)-1,4-benzenedicarbonyl dichloride and 4-(octyloxy)-1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-40-9

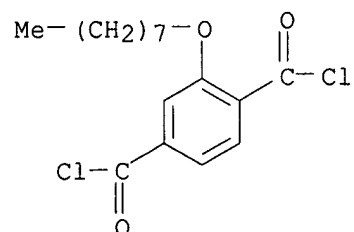
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

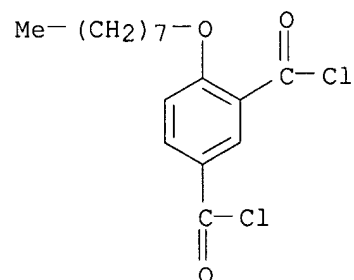
CMF C16 H20 Cl2 O3



CM 3

CRN 70065-39-3

CMF C16 H20 Cl2 O3

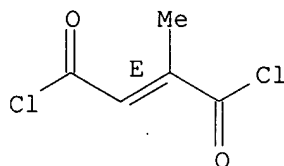


CM 4

CRN 20537-97-7

CMF C5 H4 Cl2 O2

Double bond geometry as shown.



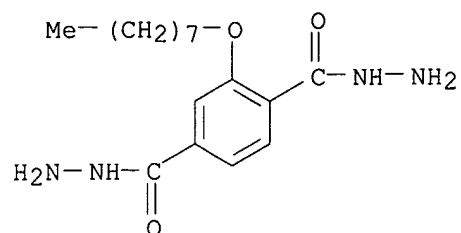
IT 651054-59-0DP, cyclodehydrated 651054-60-3DP,
cyclodehydrated 651054-61-4DP, cyclodehydrated
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and chemical-phys. characterization of unsatd.
alkoxy-substituted poly(phenylene oxadiazole)s)

RN 651054-59-0 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with
(2E)-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl
dichloride (9CI) (CA INDEX NAME)

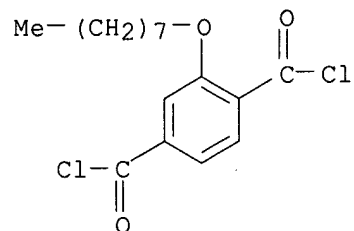
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

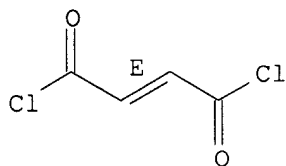
CRN 321588-70-9
CMF C16 H20 Cl2 O3



CM 3

CRN 627-63-4
CMF C4 H2 Cl2 O2

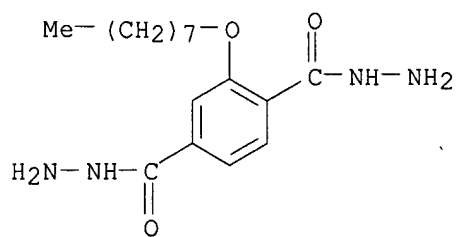
Double bond geometry as shown.



RN 651054-60-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with
(2E)-2-methyl-2-butenedioyl dichloride and 2-(octyloxy)-1,4-
benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

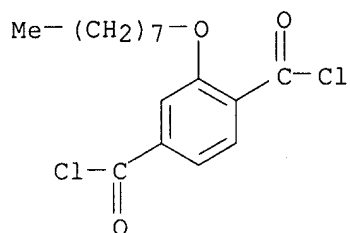
CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

CMF C16 H20 C12 O3

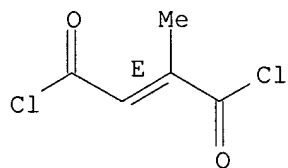


CM 3

CRN 20537-97-7

CMF C5 H4 C12 O2

Double bond geometry as shown.



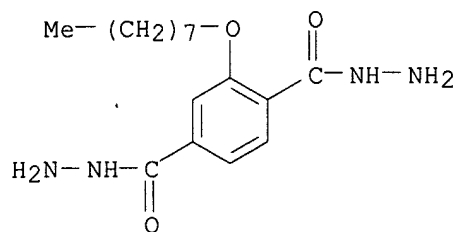
RN 651054-61-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride, 2-(octyloxy)-1,4-benzenedicarbonyl dichloride and 4-(octyloxy)-1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-40-9

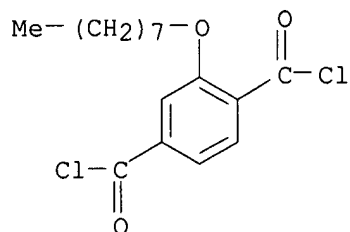
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9

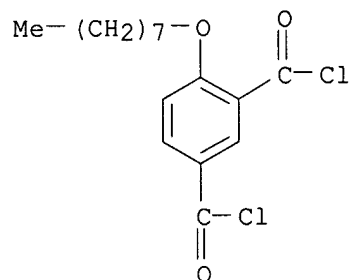
CMF C16 H20 Cl2 O3



CM 3

CRN 70065-39-3

CMF C16 H20 Cl2 O3

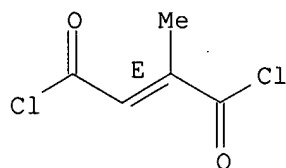


CM 4

CRN 20537-97-7

CMF C5 H4 Cl2 O2

Double bond geometry as shown.



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2003:551374 CAPLUS

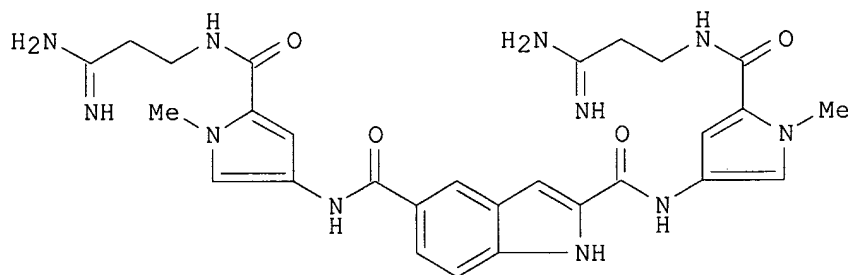
DN 139:117331

TI Preparation of polyamide analogs possessing antibacterial, antifungal, and/or antitumor activity

IN Dyatkina, Natalia B.; Shi, Dong-fang; Roberts, Christopher Don; Velligan, Mark Douglas; Liehr, Sebastian Johannes Reinhard; Botyanszki, Janos; Zhang, Wentao; Khorlin, Alexander; Nelson, Peter Harold; Muchowski, Joseph Martin

PA Genelabs Technologies, Inc., USA; et al.
 SO PCT Int. Appl., 174 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|--|----------|-----------------|----------|
| PI | WO 2003057212 | A1 | 20030717 | WO 2002-US41087 | 20021224 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| | AU 2002364209 | A1 | 20030724 | AU 2002-364209 | 20021224 |
| | US 2003212113 | A1 | 20031113 | US 2002-328710 | 20021224 |
| | US 7064218 | B2 | 20060620 | | |
| | BR 2002007583 | A | 20040427 | BR 2002-7583 | 20021224 |
| | NO 2003003773 | A | 20031023 | NO 2003-3773 | 20030825 |
| PRAI | US 2001-343796P | P | 20011226 | | |
| | US 2001-343829P | P | 20011226 | | |
| | WO 2002-US41087 | W | 20021224 | | |
| OS | MARPAT 139:117331 | | | | |
| GI | | | | | |



I

AB Compds. of formula $R1Z1COX1NHCOX2CONHX3COZ2R2$ [wherein Z1 and Z2 = independently NR3, O; R3 = H, alkyl; R1 and R2 = independently substituted alkyl or aryl, (un)substituted heteroaryl; X2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X1 and X3 = independently (un)substituted aryl or heteroaryl, CHR4; R4 = (un)natural amino acid side chain; or their pharmaceutically acceptable salts] were prepared as topoisomerase inhibitors (no data) for use as antibacterial, antifungal, and/or antitumor agents. For example, 1H-indole-2,5-dicarboxylic acid dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid [2-(carbamimidoyl)ethyl]amide in DMF to give I. Compds. of the invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of $<45.5 \mu M$. DNA binding assays showed that invention compds. bind to DNA very tightly, with apparent $K_{d,app}$ values below 100 nM for most compds. tested.

IT 386253-05-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

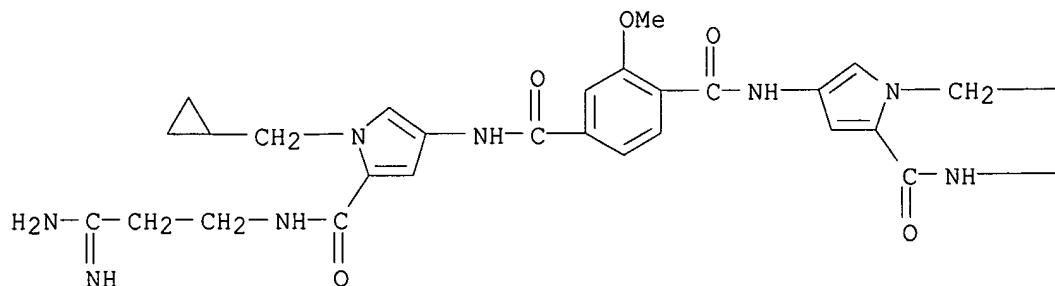
(Uses)

(drug candidate; preparation of polyamides as antibacterial, antifungal, and/or antitumor agents)

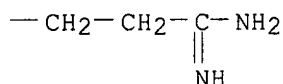
RN 386253-05-0 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis[5-[[3-amino-3-
iminopropyl)amino]carbonyl]-1-(cyclopropylmethyl)-1H-pyrrol-3-yl]-2-
methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



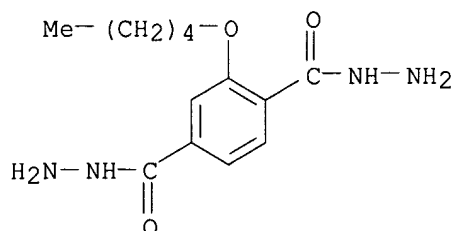
PAGE 1-B



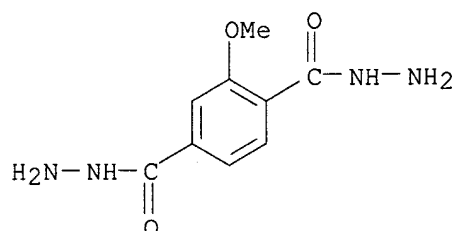
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:881449 CAPLUS
DN 138:145393
TI Synthesis and liquid crystalline properties of low molecular mass
compounds containing the 1,4-bis(5-phenyl-1,3,4-oxadiazolyl)benzene unit
AU Acierno, Domenico; Concilio, Simona; Diodati, Angela; Iannelli, Pio;
Piotto, Stefano P.; Scarfato, Paola
CS Dipartimento di Ingegneria dei Materiali e della Produzione, Universita di
Napoli, Naples, I-80125, Italy
SO Liquid Crystals (2002), 29(11), 1383-1392
CODEN: LICRE6; ISSN: 0267-8292
PB Taylor & Francis Ltd.
DT Journal
LA English
AB The synthesis and characterization of low mol. mass compds. containing
1,4-bis(5-phenyl-1,3,4-oxadiazolyl)benzene is reported. All compds. are
fluorescent in solution Due to the flat shape of the conjugated unit,
smectic-like packing is observed at high temps. for some of the synthesized
compds. Also the insertion of a lateral flexible alkoxy unit strongly
destabilizes the smectic order while promoting the appearance of a nematic
phase in the case of the shortest methoxy unit. The mesogenic character
of this unit may be of interest in the synthesis of liquid crystalline
polymeric
systems, taking advantage of both the fluorescent properties and the
peculiar mol. structure of the liquid crystalline state.

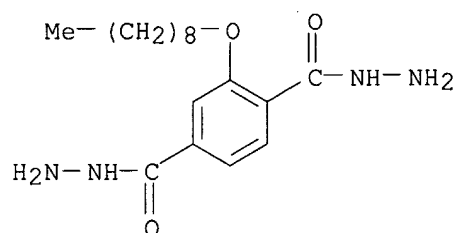
IT 428516-39-6P, Pentyloxyterephthalic dihydrazide
 492458-31-8P, Methoxyterephthalic dihydrazide 492458-32-9P
 , Nonyloxyterephthalic dihydrazide
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and esterification of)
 RN 428516-39-6 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide (9CI) (CA INDEX
 NAME)



RN 492458-31-8 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-methoxy-, dihydrazide (9CI) (CA INDEX
 NAME)



RN 492458-32-9 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-(nonyloxy)-, dihydrazide (9CI) (CA INDEX
 NAME)



RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2002:234092 CAPLUS
 DN 136:402117
 TI Alkoxy-Substituted Poly(p-phenylene 1,3,4-oxadiazole)s: Synthesis,
 Chemical Characterization, and Electro-Optical Properties
 AU Gillo, M.; Iannelli, P.; Laurienzo, P.; Malinconico, M.; Roviello, A.;
 Mormile, P.; Petti, L.
 CS Istituto di Chimica e Tecnologia dei Polimeri (ICTP)-CNR, Pozzuoli, Naples,
 34-80078, Italy
 SO Chemistry of Materials (2002), 14(4), 1539-1547

CODEN: CMATEX; ISSN: 0897-4756

PB American Chemical Society

DT Journal

LA English

AB The synthesis of a series of conjugated aromatic polyoxadiazoles (PODn) characterized by having moderate chain flexibility and highly flexible lateral substituents is reported. The majority of these polymers are soluble in a mixture of chloroform and trifluoroacetic acid and have inherent viscosities up to 0.9 dL/g. The glass transition temperature, T_g , lies in the range 165-230 °C and depends on the side-chain length. The PODn show a good thermal stability in nitrogen up to 270°C. Wide-angle X-ray diffractograms reveal a "comblake" organization of the polymeric chains. Homogeneous thin films of such a material were prepared by the spin-coating technique. Films spun on fused silica were characterized by spectroscopic anal. in the whole UV-vis-NIR range showing a high transmission in the NIR region which is the typical telecommunication band (1300-1500 nm). Furthermore, the refractive index and the film thickness have been measured using the coupled modes technique in a planar guiding structure having POD as the core. A device was prepared consisting of the said polymer sandwiched between two electrodes on top of a glass substrate. The electron conductivity of the polymer has been found to be

higher

than that of terephthalic poly(1,3,4-oxadiazole).

IT 428516-42-1P 428516-43-2P 428516-44-3P

428516-45-4P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(synthesis, chemical characterization, and electro-optical properties of alkoxy-substituted poly(p-phenylene-1,3,4-oxadiazoles))

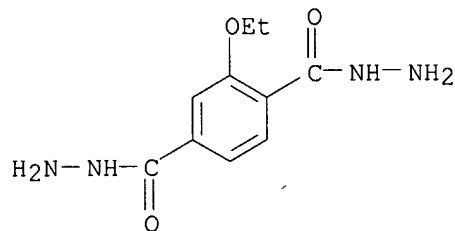
RN 428516-42-1 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-ethoxy-, dihydrazide, polymer with 2-ethoxy-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

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CRN 428516-38-5

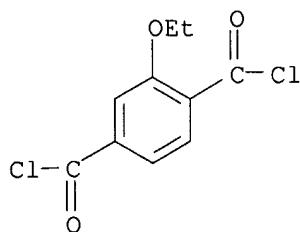
CMF C10 H14 N4 O3



CM 2

CRN 321588-61-8

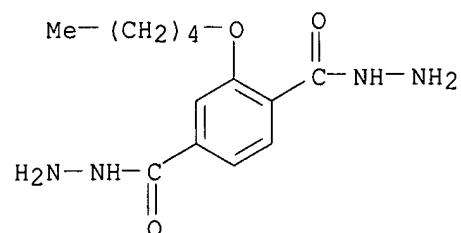
CMF C10 H8 Cl2 O3



RN 428516-43-2 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide, polymer with
2-(pentyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

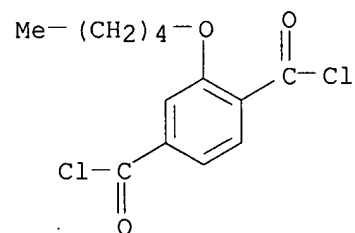
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CRN 428516-39-6
CMF C13 H20 N4 O3



CM 2

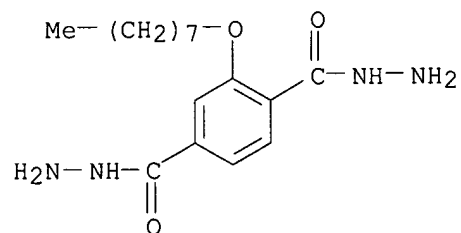
CRN 193150-89-9
CMF C13 H14 Cl2 O3



RN 428516-44-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with
2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

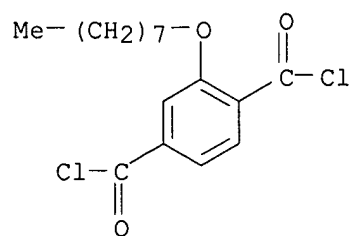
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9
CMF C16 H20 Cl2 O3



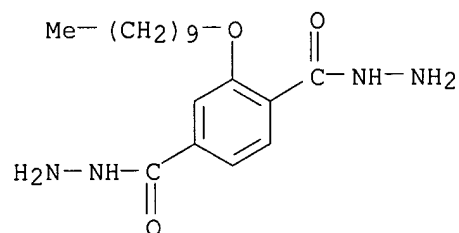
RN 428516-45-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(decyloxy)-, dihydrazide, polymer with 2-(decyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 428516-41-0

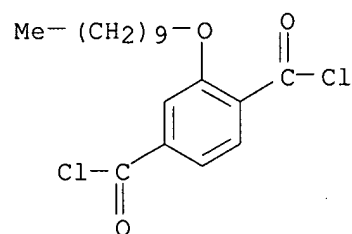
CMF C18 H30 N4 O3



CM 2

CRN 321588-74-3

CMF C18 H24 C12 O3



IT 428516-38-5P 428516-39-6P 428516-40-9P

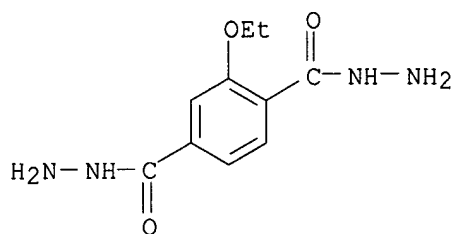
428516-41-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

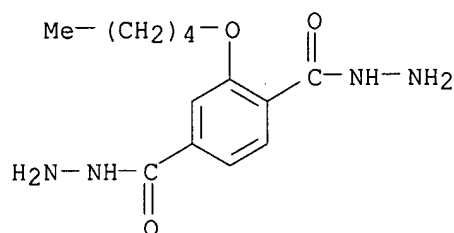
(synthesis, chemical characterization, and electro-optical properties of alkoxy-substituted poly(p-phenylene-1,3,4-oxadiazoles))

RN 428516-38-5 CAPLUS

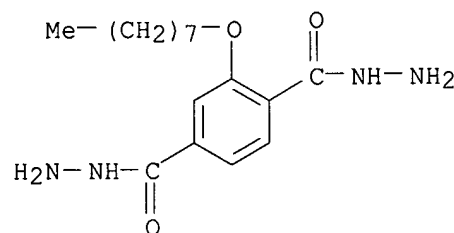
CN 1,4-Benzenedicarboxylic acid, 2-ethoxy-, dihydrazide (9CI) (CA INDEX NAME)



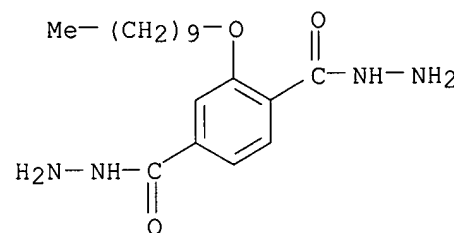
RN 428516-39-6 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RN 428516-40-9 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RN 428516-41-0 CAPLUS
 CN 1,4-Benzenedicarboxylic acid, 2-(decyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2002:10469 CAPLUS
 DN 136:85750
 TI Preparation of novel compounds possessing antibacterial, antifungal or
 antitumor activity
 IN Zhang, Wentao; Liehr, Sebastian Johannes R.; Velligan, Mark Douglas;

Dyatkina, Natalia B.; Botyanszki, Janos; Shi, Dong-Fang; Roberts, Christopher Don; Khorlin, Alexander; Nelson, Peter Harold; Muchowski, Joseph Martin

PA Genelabs Technologies, Inc., USA

SO PCT Int. Appl., 141 pp.

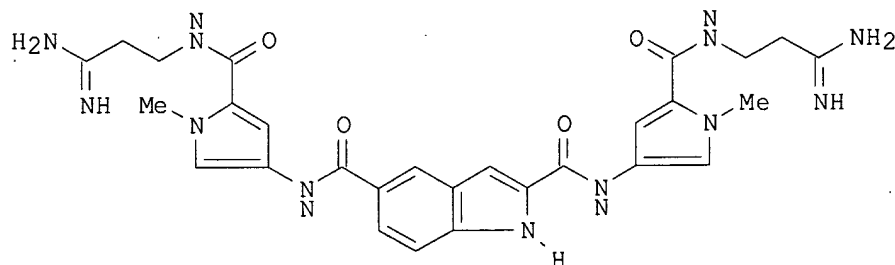
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 2002000650 | A2 | 20020103 | WO 2001-US20334 | 20010626 |
| | WO 2002000650 | A3 | 20021024 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2414512 | A1 | 20020103 | CA 2001-2414512 | 20010626 |
| | US 2002037856 | A1 | 20020328 | US 2001-892327 | 20010626 |
| | US 6849713 | B2 | 20050201 | | |
| | EP 1294713 | A2 | 20030326 | EP 2001-948740 | 20010626 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| | BR 2001012030 | A | 20030429 | BR 2001-12030 | 20010626 |
| | JP 2004501915 | T | 20040122 | JP 2002-505774 | 20010626 |
| | NZ 522839 | A | 20041126 | NZ 2001-522839 | 20010626 |
| | US 2003119749 | A1 | 20030626 | US 2002-277666 | 20021023 |
| | US 6906103 | B2 | 20050614 | | |
| | NO 2002005720 | A | 20030226 | NO 2002-5720 | 20021128 |
| | ZA 2002009774 | A | 20040302 | ZA 2002-9774 | 20021202 |
| | MX 2002PA12271 | A | 20040906 | MX 2002-PA12271 | 20021211 |
| PRAI | US 2000-214478P | P | 20000627 | | |
| | US 2001-892327 | A3 | 20010626 | | |
| | WO 2001-US20334 | W | 20010626 | | |
| OS | MARPAT 136:85750 | | | | |
| GI | | | | | |



AB Compds. of formula $R_1Z_1COX_1NHCOX_2CONHX_3COZ_2R_2$ (Z_1 and Z_2 = independently NR_3 , O; R_3 = H, alkyl; R_1 and R_2 = independently substituted alkyl or aryl, (un)substituted heteroaryl; X_2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X_1 and X_3 = independently (un)substituted aryl or heteroaryl, CHR_4 ; R_4 = (un)natural amino acid side chain) or their pharmaceutically acceptable salts were prepared and possess one or more of the following activities: antibacterial, antifungal and antitumor activity. For example, 1H-Indole-2,5-dicarboxylic acid

dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid (2-carbamimidoyl-ethyl)-amide in DMF to give compound I. Comps. of this invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of <45.5 μ M. Studies of their DNA binding properties demonstrated that they bind to DNA very tightly, with apparent K_d , app values below 100 nM for most comps. tested.

IT 386253-05-0P

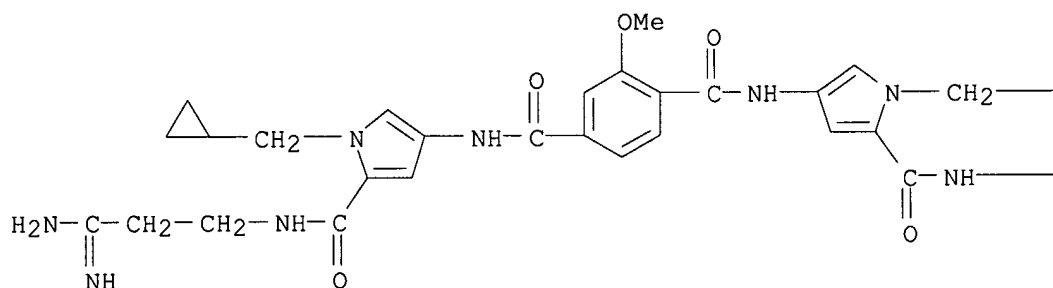
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel comps. possessing antibacterial, antifungal or antitumor activity)

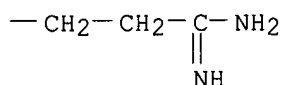
RN 386253-05-0 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis[5-[[[3-amino-3-iminopropyl)amino]carbonyl]-1-(cyclopropylmethyl)-1H-pyrrol-3-yl]-2-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L3 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2001:403466 CAPLUS

DN 135:24726

TI Polymerizable compositions containing aromatic amide group-containing (meth)acrylic monomers and dental restorative materials

IN Yamakawa, Junichiro; Kazama, Hideki

PA Tokuyama Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|----------------|------|----------|-----------------|----------|
| PI | JP 2001151808 | A | 20010605 | JP 1999-335874 | 19991126 |
| PRAI | JP 1999-335874 | | 19991126 | | |

AB The comps., which show high fracture toughness and can be substitutes for

metal materials, comprise (A) monomers containing $R_1(\text{CONHR}_2\text{COCR}_3\text{CH}_2)_n$ [R_1 = mono-, di-, or trivalent C6-24 organic group having 1-3 aromatic ring selected from benzene, naphthalene, and anthracene; R_2 = (CB1B2) k A1, (CB1B2) k A1COR4[(CH2)1A2] m , (CB1B2) k A1COR4A2, (CB1B2) k A1COR4CO[(CH2)1A2] m , (CB1B2) k A1[(CH2)1A2] m (A1, A2 = O, NH; B1, B2 = H, C1-5 alkyl, C1-5 alkoxy, Ph; R4 = C1-12 hydrocarbylene; k, l, m = 1-5)], (B) fillers containing 40-99% approx. spherical inorg. particles having average particle size 0.1-5 μm and 1-60% inorg. particles having average particle size 0.01-0.1 μm , and (C) polymerization initiators. The compns. may addnl. contain 10-300 parts [based on 100 parts (B)] amorphous inorg. particles which have average particle size 0.1-9 μm and contain $\leq 3\%$ those having particle size $\geq 10 \mu\text{m}$. Dental restorative materials comprising the composition are also claimed. A composition containing

1,3-C6H4(CONHCH2CH2OCOC6H4CO2CH2CH2OCOC

Me:CH2-3)2 (I) 60, triethylene glycol dimethacrylate 40, 60:40 mixture of spherical SiO2-ZrO2 filler (average particle size 0.52 μm) and spherical SiO2-TiO2 filler (average particle size 0.08 μm) 400, and bis(2,4,6-trimethylbenzoyl)phenylphosphine oxide 0.05 part was irradiated with light and heated at 100° for 20 min to give a cured sample. Fracture toughness of the cured sample 24 h after soaking in H2O at 37° was 3.3 MPa.m^{1/2}, vs. 2.3 MPa.m^{1/2} for a control prepared from a composition containing Bis-GMA instead of I.

IT 342902-75-4P

RL: PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polymerizable dental composite resin compns. containing aromatic amide group-containing (meth)acrylic monomers for high fracture strength)

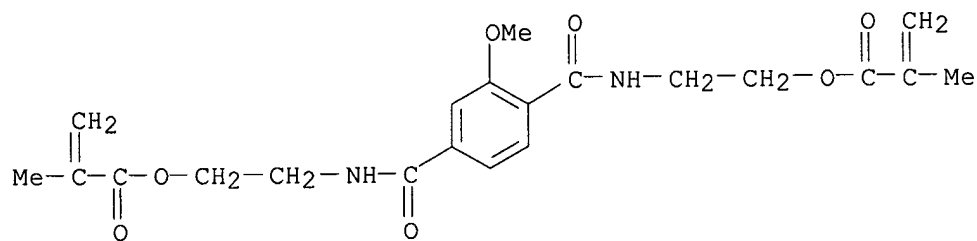
RN 342902-75-4 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester, polymer with (2-methoxy-1,4-phenylene)bis(carbonylimino-2,1-ethanediyl) bis(2-methyl-2-propenoate) (9CI) (CA INDEX NAME)

CM 1

CRN 342902-74-3

CMF C21 H26 N2 O7



CM 2

CRN 109-16-0

CMF C14 H22 O6

